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Dislocation-mediated strain hardening in tungsten: Thermo-mechanical plasticity theory and experimental validation

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ABSTRACT

A self-consistent thermo-mechanical model to study the strain-hardening behavior of polycrystalline tungsten was developed and validated by a dedicated experimental route. Dislocation–dislocation multiplication and storage, as well dislocation-grain boundary (GB) pinning were the major mechanisms underlying the evolution of plastic deformation, thus providing a link between the strain hardening behavior and material's microstructure. The microstructure of the polycrystalline tungsten samples has been thoroughly investigated by scanning and electron microscopy. The model was applied to compute stress–strain loading curves of commercial tungsten grades, in the as-received and as-annealed states, in the temperature range of 500–1000 °C. Fitting the model to the independent experimental results obtained using a single crystal and as-received polycrystalline tungsten, the model demonstrated its capability to predict the deformation behavior of as-annealed samples in a wide temperature range and applied strain. The relevance of the dislocation-mediated plasticity mechanisms used in the model have been validated using transmission electron microscopy examination of the samples deformed up to different amounts of strain. On the basis of the experimental validation, the limitations of the model are determined and discussed.

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1. Introduction

The response of structural or functional materials to impact, cyclic or shock mechanical or thermal loading conditions is of practical concern for a variety of nowadays applications, including structural crashworthiness, ballistic events, and explosive–structure interactions. Often, materials owing the needed properties are heterogeneous or at least exhibit a complex microstructure, if considered at the micro-scale, for example polycrystalline metals, fiber reinforced composites, metallic laminates (see e.g. [1,2]). Modern computational science dealing with plasticity phenomenon underlines a role played by

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dislocations and GBs which practically define the trans-granular (i.e. at nano- to micro-scale level) and inter-granular (at micro- to meso-scale level) plastic deformation (see e.g. [3,4]). Hence, desirable mechanical properties of a certain metallic matrix for extreme applications can be achieved by optimizing its microstructure. That is why many efforts are currently put on the exploration of the relationship of microstructure and mechanical response to gain physical understanding implantable in the fast developing computational models (see e.g. [5,6]).

The international program on thermonuclear fusion is one of the examples, where the application of materials in extreme environmental conditions cannot be avoided [7]. Refractory metals, and in particular tungsten (W) is one of the materials that will play an important role in the ITER as well as in DEMO projects [8–10]. It is a promising plasma facing material for both the divertor and the first wall because of its high melting temperature and resistance to sputtering by low-energy ions. An important general drawback for structural applications is a relatively low ductile-to-brittle transition temperature (DBTT) of W around 300–400 °C [11]. This transition appears to be controlled by dislocation mobility and microstructural features limiting their multiplication and storage.

Indeed, Brunner and co-workers have been intensively involved in the study of mechanical properties of pure tungsten (W), including both single- and polycrystals. A series of experimental work have been performed to study the plastic properties of high-purity tungsten single crystals [12–14]. It was indicated that the appearance of the work hardening mode in tungsten single crystals is closely related to the transition temperature being $(0.1–0.2)T_m$ (the melting point temperature), being dominated by the mobility of screw dislocations [14]. The compression tests, done in pure polycrystalline tungsten in a wide temperature range, revealed a surprisingly moderate ductility [15]. As what concerns the theoretical study of the thermo-mechanical behavior of polycrystalline tungsten, both phenomenological and physically-based models can be found in literature (see e.g. [15,16]), where the major element ensuring plasticity is defined as the thermally activated motion of screw dislocations. However, the mentioned above works put focus on the yield phenomena and therefore considered low temperature interval (below $0.2T_m$), where the strain hardening of polycrystalline tungsten is limited.

For high temperature applications, such as the divertor or armor plates in ITER, the thermal cyclic fatigue and re-crystallization are important issues [17]. The deterioration effect of neutron irradiation and plasma uptake comes on the top of the thermal stresses induced by the plasma instabilities.

For a better understanding of the material response to the thermal cyclic load, it is essential to develop physically based approaches integrated into computational codes at the aggregate level to ensure the integrity and optimum performance of fusion reactor components [18]. It is well recognized that fracture as a physical phenomenon is controlled by a series of processes ranging from the atomic scale to the grain-size scale and beyond. At a mesoscopic scale, the determination of the stress/strain fields around a crack tip is of primary importance and finite element (FE) analysis is widely used for the assessment of the mechanical response to external load [4,16]. The inherent feature of any FE computation is the so-called constitutive laws, i.e., the stress–strain relationship of a representative volume element.

In our previous work, we have studied the strain-hardening behavior of commercial tungsten grades in temperature range 500–2000 °C [19], in the frame of a phenomenological model describing the evolution of flow stress as a function of dislocation density [20]. The strain-hardening behavior was sub-divided onto three types depending on test temperature: (i) below 1000 °C, the main source of strain-hardening was the dislocation–interface interaction (low angle GBs in as-received due to forging or hammering and random GBs in as-annealed materials); (ii) at 1000–1500 °C, the pinning of dislocations was assigned to be controlled by random GBs mainly; and (iii) at 1500 °C and above intensive in-situ creep was observed. However, that oversimplified model, based on the two-parameter Kocks and Mecking approach for dislocation density evolution, assumed that the defect density and spacing obstructing dislocation motion remains constant in the course of plastic deformation as well as the model treated the material as medium without any distinction between grains and subgrains. The latter simplification might be an important limiting factor when it comes to channel deformation or grain-boundary slip. Recently, a role played by a bi-modal grain size distribution in the plastic deformation was addressed by Berbenni et al. [21] using the crystal plasticity framework. The latter demonstrated a strong impact of grain size dispersion on strain-hardening capacity and ductility especially with the reduction of the sub-grain size to several microns, while the random grain size is by a factor of 10 to 20 higher, which is relevant grain size distribution for commercial heavily forged tungsten grades. Another important limitation of the model is its incapability to treat the irradiation induced hardening due to the lattice defects which experience modification of their properties as plastic flow progresses (the absorption and transformation of dislocation loops in BCC metals [22] and stacking fault tetrahedral in FCC metals [23] are well known phenomena). Hence, further development of the crystal plasticity model for polycrystalline tungsten is needed to overcome the above mentioned shortcomings.

In this work, we continue the investigation of the strain-hardening behavior by using a recently developed self-consistent thermo-mechanical model [24]. The model was originally developed for FCC copper and was successfully applied to describe not only the temperature effects but also neutron irradiation defects affecting the strain-hardening response. The model therefore can treat both effects of irradiation defects and pre-existing microstructures accounting for the stress-thermal activation proving dislocation-mediated slip. While the thermal activation effects are treated at the grain level by means of a tensorial plasticity crystal model, the elastic–viscoplastic self-consistent approach [25–28] is applied for the scale transition from individual grains to macroscopic polycrystalline. Here, we applied this model to treat the stress–strain behavior of commercial polycrystalline tungsten grades in the as-received (i.e. heavily plastically deformed) and annealed states. A unique parameterization set is designed and found to predict well both yield stress and work-hardening regime in the temperature range 773–1273 K (i.e. 500–1000 °C), as above it the role of creep in the course of standard tensile test is

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