Numerical investigation of the brittle-to-ductile transition temperature of rolled high-purity tungsten

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Numerical investigation of the brittle-to-ductile transition temperature of rolled high-purity tungsten

M.A. Oude Vrielink , J.A.W. van Dommelen, M.G.D. Geers

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Highlights

- Predictive model for the constitutive behaviour of tungsten in the BDTT range.
- Statistically well-defined brittle cleavage criterion is proposed.
- Accurate simulation results for the prediction of the BDTT of high purity tungsten.
- The anisotropic BDTT of rolled tungsten is in line with experimental results.
- Realistic values of the strain rate dependency of the BDTT are obtained.

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Numerical investigation of the brittle-to-ductile transition temperature of rolled high-purity tungsten

M.A. Oude Vrielink, J.A.W. van Dommelen*, M.G.D. Geers

Department of Mechanical Engineering, Eindhoven University of Technology.

Abstract

With increasing temperature, high-purity tungsten typically shows a sharp transition from fully brittle behaviour to a significantly more ductile response. The brittle-to-ductile transition of tungsten is not an invariant property, but depends on the microstructure and loading conditions. In the current work, this relation is investigated numerically. To this end, a crystal plasticity framework is adopted, combined with a newly proposed cleavage criterion. The crystal plasticity parameters are identified from experimental data, obtained from tensile tests on rolled polycrystalline samples. The brittle-to-ductile transition is subsequently examined for different strain rates, which allows for calculating the activation energy of the brittle-to-ductile transition. The resulting activation energy is in adequate agreement with experimental findings in literature. Finally, different loading directions with respect to the anisotropic microstructure are considered. The numerically obtained transition temperatures in these directions are consistent with experimental data. The proposed model is therefore instrumental for improving the design of the tungsten monoblocks for future fusion reactors.

Keywords: Crystal plasticity, tungsten, brittle-to-ductile transition, activation energy

1. Introduction

Nuclear fusion has the potential to provide a practically limitless amount of relatively safe and clean energy. During the fusion process, hydrogen isotopes are fused together to form helium, which releases a tremendous amount of energy. The process occurs at extremely high temperatures, causing the particles to behave as a plasma. In order to exploit this type of energy generation, a fusion reactor must withstand extreme conditions. Plasma facing components are subjected to large heat flows, and are heavily bombarded with ions and neutrons. Tungsten has a number of favourable material properties compared to other materials, including a high melting temperature, high thermal conductivity, and a low sputtering yield. To this end, pure tungsten is proposed as armour material for the plasma facing components in future nuclear fusion reactors [1]. Since the tungsten components are subjected to an extreme heat-loading and simultaneously actively (water-)cooled, a huge temperature gradient arises causing stresses in the material. While the operating temperature of pure tungsten has an upper limit due to issues such as melting and possibly recrystallization, it also has a marked lower limit due to its sharp transition in failure behaviour. Here, the mechanism changes from ductile fracture to brittle cleavage [2–7], which is a sharp and sudden transition that is undesirable.

In this work, a numerical approach is used to investigate the brittle-to-ductile transition of tungsten. The temperature at which this transition occurs is not an intrinsic material property; it depends on the microstructure and loading conditions [3–5, 7]. The plasma facing components should therefore be designed such that failure due to this phenomenon is avoided. Related work in literature that focusses on the modelling of the brittle-to-ductile transition temperature of high purity tungsten relies on crack-tip plasticity by means of discrete dislocation dynamics [3, 8]. Here, typically only one or a few crystals are considered, which makes these methods less suitable to investigate the influence of texture of a whole

*Corresponding author

Email address: J.A.W.v.Dommelen@tue.nl (J.A.W. van Dommelen)

aggregate. The current work aims to obtain direct insight on the influence of the microstructure on the brittle-to-ductile transition.

The ductile response of tungsten is modelled in a crystal plasticity framework. In the low temperature regime, tungsten has a strongly decreasing yield stress with increasing temperature due to its body-centred-cubic stacking. This type of stacking leads to a high Peierls stress emanating from the screw dislocations that govern plasticity in this material. The slip resistance in this work therefore includes a term that results from the activation energy of kink-pair formation in screw dislocation lines. This modelling approach was presented earlier by Weinberger et al. [9] and Lim et al. [10]. In order to model fracture, a novel Rankine-type (temperature and strain rate independent) cleavage criterion is included, that is statistically well defined. In the current work, fracture is considered to be brittle if it occurs at a macroscopic tensile strain below 1%, and ductile otherwise. The temperature at which the strain-to-failure equals 1% is identified as the brittle-to-ductile transition temperature. This approach allows to numerically assess the brittle-to-ductile transition temperature for an aggregate of tungsten crystals. The numerical model supporting this analysis allows to identify the most important factors governing the brittle-to-ductile transition. It is therefore expected to be instrumental in improving the design of the tungsten monoblocks.

The outline of the paper is as follows. In section 2, the material model is described. The model for the slip rate includes a temperature-dependent kink-pair slip resistance. In section 3, the model parameters are identified from experimental data, obtained from tensile experiments on polycrystalline tungsten microstructures. In section 4, a new cleavage criterion is introduced, after which the brittle-to-ductile transition temperature is identified in section 5. Different loading directions with respect to the anisotropic microstructure are also considered. The paper is finalised by a discussion in section 6, and conclusions in section 7, which summarizes the main findings of this paper.

2. Crystal plasticity material model

In this section, the crystal plasticity modelling approach is discussed, which lines up with the work of Asaro [11]. The mechanical behaviour of the material is modelled with a rate dependent crystal plasticity formulation, which includes the elastic response and the temperature dependence of the slip systems.

2.1. Kinematics

The deformation in a material point is described by the deformation gradient tensor $\mathbf{F}$. In this model, $\mathbf{F}$ is composed of an elastic distortion $\mathbf{F}_e$ and a plastic part $\mathbf{F}_p$:

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_p . \quad (1)$$

The plastic velocity gradient tensor $\mathbf{L}_p$ is given by the sum of the contributions of the crystallographic shear rates $\dot{\gamma}^\alpha$ as

$$\mathbf{L}_p = \dot{\mathbf{F}}_p \cdot \mathbf{F}_p^{-1} \quad (2)$$

$$= \sum_{\alpha=1}^{N_s} \dot{\gamma}^\alpha \mathbf{P}_{s,0}^\alpha = \sum_{\alpha=1}^{N_s} \dot{\gamma}^\alpha \bar{s}_0^\alpha \bar{n}_0^\alpha , \quad (3)$$

with $\mathbf{P}_{s,0}^\alpha$ the non-symmetric Schmid tensor of slip system α , $\bar{s}_0^\alpha$ its slip direction and $\bar{n}_0^\alpha$ its slip plane normal. Regarding the active slip systems in body-centred cubic metal, some discrepancies exist in literature. While slip is frequently assumed to occur only on the $\{\bar{1}01\} \langle 111 \rangle$ family slip systems (see e.g. Gröger et al. [12], Weinberger et al. [9] and Cereceda et al. [13]), others assume only on the $\{112\} \langle 111 \rangle$ family of slip systems to be active (Seegeer [14, 15]), or on a combination of both (Terentyev et al. [16]). In this work, slip is assumed to occur only on the $\{\bar{1}01\} \langle 111 \rangle$ family of slip systems, and therefore the number of slip systems is $N_s = 12$.

2.2. Elastic behaviour

The elastic part of the response is described by a linear relation as

$$\mathbf{S}_e = {}^4\mathbb{C} : \mathbf{E}_e, \quad (4)$$

where ${}^4\mathbb{C}$ is the fourth-order isotropic elasticity tensor, and

$$\mathbf{S}_e = \det(\mathbf{F}_e) \mathbf{F}_e^{-1} \cdot \boldsymbol{\sigma} \cdot \mathbf{F}_e^{-T} \quad (5)$$

is the (symmetric) elastic second-order Piola-Kirchhoff stress tensor. Here, $\boldsymbol{\sigma}$ is the Cauchy stress tensor. The elastic Green-Lagrange strain tensor $\mathbf{E}_e$ is defined as:

$$\mathbf{E}_e \equiv \frac{1}{2}(\mathbf{C}_e - \mathbf{I}). \quad (6)$$

Here, $\mathbf{C}_e = \mathbf{F}_e^T \cdot \mathbf{F}_e$ is the right Cauchy-Green deformation tensor and $\mathbf{I}$ the second-order unit tensor.

2.3. Crystallographic slip

Plasticity is governed by crystallographic slip on slip systems due to dislocation nucleation and propagation. Crystallographic slip is described by a rate dependent flow rule, where the rate of slip on each of the slip-systems is dependent on the resolved shear stress as well as on the resistance to slip. To this end, a phenomenological power law relation is adopted:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{|\tau^\alpha|}{s^\alpha} \right)^{\frac{1}{m}} \text{sign}(\tau^\alpha). \quad (7)$$

Here, τ^α is the resolved shear stress on each of the slip systems $\alpha = 1, 2, \dots, N_s$, m is the strain rate sensitivity and $\dot{\gamma}_0$ is the reference slip rate. Following Kothari and Anand [17], the total resistance to slip s^α on a given slip system α is decomposed into long-range and short-range barriers; the obstacle slip resistance s_{obs}^α and the kink-pair slip resistance s_{kp}^α respectively:

$$s^\alpha = s_{\text{obs}}^\alpha + s_{\text{kp}}^\alpha. \quad (8)$$

The obstacle slip resistance s_{obs}^α increases with the amount of accumulated plastic slip and represents hardening as a consequence of dislocation entanglement and other defects. The kink-pair slip resistance s_{kp}^α is the result of the high Peierls barrier of tungsten at low temperatures.

2.3.1. Obstacle slip resistance

Dislocation propagation is hindered by obstacles such as dislocation entanglement and precipitates. The obstacle slip resistance represents the hardening of the material, and is described by the following generic formulation:

$$\dot{s}_{\text{obs}}^\alpha = \sum_{\beta} h^{\alpha\beta} |\dot{\gamma}^\beta|, \quad (9)$$

where $h^{\alpha\alpha}$ represents the self-hardening effects and $h^{\alpha\beta}$ ($\alpha \neq \beta$) represents the latent-hardening effects. The hardening coefficients are taken as:

$$h^{\alpha\beta} = (q_n + (1 - q_n) \delta^{\alpha\beta}) h^\beta, \quad (10)$$

with $\delta^{\alpha\beta}$ the Kronecker delta and q_n the interaction matrix coefficient. The hardening rate is described as

$$h^\beta = h_0 \left(1 - \frac{s_{\text{obs}}^\beta}{s_\infty} \right)^a. \quad (11)$$

Here, the asymptotic slip resistance s_∞ is the value that represents the slip resistance s_{obs} after an infinite amount of slip. This value is assumed to be temperature independent. Furthermore, h_0 is the initial hardening rate.

2.3.2. Kink-pair slip resistance

Although the obstacle slip resistance will dominate at elevated temperatures, a second source of slip resistance is non-negligible in the range of the brittle-to-ductile transition temperature. In order for dislocation lines to propagate, they should overcome the Peierls potential, which is the periodic resistance of the crystal lattice. This occurs by the formation of kink-pairs on the dislocation lines. The resistance to this kind of obstacles is thermally activated, as its contribution becomes negligible at temperatures above the so-called knee-temperature T_k^α of the slip system. Its expression is similar to the formulation given by Seeger [18]:

$$T_k^\alpha = \frac{-G_0}{k_b \ln((|\dot{\gamma}^\alpha| + \epsilon)/\dot{\gamma}_{kp,0})}; \quad (12)$$

Here, k_b is the Boltzmann constant, and $\epsilon = 10^{-8}$ is an arbitrary small value, introduced solely for numerical reasons. Furthermore, G_0 is the activation energy and $\dot{\gamma}_{kp,0}$ is the reference kink-pair slip rate. As proposed by Lim et al. [19], the subsequent expression for the kink-pair slip resistance then becomes:

$$s_{kp}^\alpha = \begin{cases} s_{kp,0} \left[1 - \left(\frac{T}{T_k^\alpha} \right)^{\frac{1}{q}} \right]^{\frac{1}{p}} & \text{if } T < T_k^\alpha \\ 0 & \text{otherwise.} \end{cases} \quad (13)$$

The exponents are typically chosen such that $0 \leq p \leq 1$ and $1 \leq q \leq 2$. As can be seen, for $T < T_k^\alpha$, the slip resistance is strain rate dependent through T_k^α . Also, the kink-pair slip resistance decreases monotonically from the reference kink-pair slip resistance $s_{kp,0}$ to 0 MPa with increasing temperature from 0 K to T_k^α .

3. Material characterization

The tungsten monoblocks for which the brittle-to-ductile transition temperature is investigated in the current work, have an anisotropic microstructure due to the rolling process used in prior manufacturing. The microscopic grains are strongly elongated in the rolling direction (RD), as indicated in figure 1. The normal direction (ND) corresponds to the direction of thickness reduction and the transverse direction (TD) is perpendicular to the ND-RD plane. Commercial high-purity tungsten samples are obtained from AT&M. The grain size of these samples is roughly 96 μm .

Figure 1: A recrystallized tungsten microstructure transforms into a new microstructure with elongated grains in a preferred direction due to rolling.

3.1. Texture

Due to the prior rolling, the crystals possess a preferred lattice orientation. In order to obtain a representative set of crystal orientations, a cross-section of a specimen is considered. An EBSD scan is performed over an area of $1000 \times 1000 \mu\text{m}$ in the TD-ND plane. From here, an orientation distribution function (ODF) is obtained, see figure 2a.

In order to perform crystal plasticity simulations with a comparable ODF, a representative set of orientations is constructed. To this end, 2500 random orientations are generated and compared to the ODF that is obtained from the scan. The 576 best-matching orientations are adopted in the subsequent simulations used in the remainder of this work. The representative set adequately matches the original ODF, as can be seen in figure 2b.

Figure 2: The pole figures of the orientation distribution function (ODF) is shown in the TD-ND plane. The ODF of a representative set composed of a smaller set of 576 grains is presented, adequately matching the original ODF.

3.2. Material parameters from literature

All parameters in the material model have a physical basis, as highlighted before. A complete integral set of the corresponding values of these parameters has not been reported in just one paper only. Therefore, the material parameters of the separate aspects of the model are obtained by exploring several sources in literature. The parameters are determined as follows. The strain rate sensitivity parameter m in the slip law is taken from Asaro [11]:

$$m = 0.02 . \quad (14)$$

Note that Wei and Kecskes [20] found very similar values for the strain rate sensitivity from experiments for different rolling conditions. Brunner [21] carried out tensile experiments on single crystal high-purity samples, and identified three different temperature regimes, where the brittle-to-ductile transition temperature is expected to be in regime II (which corresponds to $220 < T < 750$ K). The activation energy G_0 from Brunner [21] in this regime is adopted in the current work:

$$G_0 = 1.75 \text{ eV} . \quad (15)$$

Since for tungsten it holds that $2c_{44} \approx c_{11} - c_{12}$, the material is assumed to be isotropic. The bulk modulus κ and shear modulus G , required to construct the elasticity tensor ${}^4\mathbb{C}$, are taken from Lowrie and Gonas [22]:

$$\kappa = 309 \text{ GPa} , \quad G = 161 \text{ GPa} . \quad (16)$$

For simplicity, the temperature dependence of these parameters is neglected in the current analysis. The underlying potential of the kink-pair slip resistance resembles the line-tension model, which is a close approximation of the more sophisticated formulations such as the Eshelby potential or the sinusoidal potential [23]. Therefore, the exponents p and q are chosen such that

$$p = 0.8 , \quad q = 1.2 . \quad (17)$$

Lim et al. [19] identified several parameters from the single-crystal data from Brunner [21], including the reference kink-pair slip rate, which is also adopted here:

$$\dot{\gamma}_{\text{kp},0} = 3.71 \cdot 10^{10} \text{ s}^{-1} . \quad (18)$$

Regarding the parameters that correspond to the hardening slip resistance, the hardening exponent a is adopted from Yalçinkaya [24] and the interaction matrix coefficient q_n is taken from Asaro [11]:

$$a = 1.5, \quad q_n = 1.4. \quad (19)$$

The remaining parameters are obtained by identification on the basis of experimental data, as shown in the next section.

3.3. Comparison to tensile-data from literature

The crystal orientations as described in section 3.1 are randomly assigned to the grains in a representative volume element (RVE). A preliminary analysis indicated that the geometry of the grains does not have a significant influence on the average mechanical response. Although grain morphology may cause local stress concentrations, the collective stress state of an assembly of grains is hardly influenced. Accordingly, the geometry the grains is taken cubic, i.e. the RVE consists of a cubic grid of 24 by 24 grains. Hence, 576 grains (and crystal orientations) are used. Another preliminary analysis indicated that a single layer of grains in the thickness direction is sufficient to describe the mechanical response of the RVE while loading perpendicular to the thickness direction. Furthermore, the RVE is discretized in a grid-like fashion, with 72 by 72 elements. Therefore, each grain consists of 3 by 3 elements, which is sufficient in order to obtain mesh convergence. Note that mesh convergence is reached rapidly, because only grain-averaged quantities are considered here. The thickness direction is meshed with a single layer of elements. The elements are (quadratic) serendipity brick-elements with reduced integration (8 integration points).

In the current work, three different RVEs (A, B and C) are investigated. The meshes of these RVEs are visualized in figure 3. The colors of each of the elements represent their crystal orientation in ND, according to the legend shown at the right. The arrows connected to the RVEs represent prescribed displacements. Black arrows indicate a prescribed displacement of zero, while the orange, green and blue arrows indicate uniaxial tensile loading at a constant strain rate. Furthermore, periodic boundary conditions are imposed in three dimensions.

Figure 3: Visualization of the three RVEs. The element colors indicate their respective crystal orientation. The black arrows indicate a prescribed displacement of zero. The orange, green and blue arrows indicate uniaxial tensile loading in TD, ND and RD, respectively. Finally, three dimensional periodic boundary conditions are imposed as well.

A full-field homogenization approach is adopted in order to obtain the macroscopic response of the polycrystalline microstructure. To this end, the macroscopic first Piola-Kirchhoff stress (force per unit of area in the reference configuration) is obtained as

$$\bar{\mathbf{P}} = \langle \mathbf{P}(\vec{x}) \rangle_{V_{\text{RVE}}}, \quad (20)$$

where vector $\vec{x}$ is the microscopic position vector in the RVE and $\langle \bullet \rangle_V$ denotes the volume averaging operator over the volume V . The macroscopic stress response of RVE B as function of the engineering strain is shown in figure 4 for loading in two different directions. Here, the response is compared to experimental data at different temperatures. Note that regarding the experimental data, only the response up to 15% strain is shown here. To this end, the reference slip rate parameter $\dot{\gamma}_0$ is taken to be equal to the applied strain rate of the characterization experiments, i.e.:

$$\dot{\gamma}_0 = 10^{-3} \text{ s}^{-1}. \quad (21)$$

The hardening parameters are identified from the experimental data. The initial hardening rate h_0 , the initial obstacle slip resistance $s_{\text{obs},0}$ and saturation slip resistance s_∞ are identified as:

$$h_0 = 3.0 \text{ GPa} , \quad s_{\text{obs},0} = 170 \text{ MPa} , \quad s_\infty = 210 \text{ MPa} . \quad (22)$$

Furthermore, it is found that the kink-pair slip resistance extrapolated to $T = 0 \text{ K}$ is

$$s_{\text{kp},0} = 600 \text{ MPa} . \quad (23)$$

In figure 4a, the black solid lines represent the numerical engineering stress as function of the engineering strain. Here, the RVE is loaded at a strain rate of $\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$ in RD at various temperatures in the range of $150 \leq T \leq 500 \text{ }^\circ\text{C}$. Clearly, the yield stress decreases with increasing temperature. The coloured dots represent the tensile data as presented by Shen et al. [25]. They performed tensile tests on high-purity tungsten with an average grain size of about $140 \times 330 \times 40 \text{ }\mu\text{m}$. In figure 4b, similar experiments are presented, but now the specimen are loaded in TD. Again, the coloured dots represent the tensile data provided by Shen et al. [25] (up to 15% engineering strain), whereas the black solid lines represent the numerical results. Figure 4 reveals that the overall macroscopic behaviour is adequately captured by the numerical model in both RD and TD. Note that the softening behaviour originates from localization of strain, which is classified as a geometrical effect. The softening does not originate from the material behaviour, and should therefore not be included in the material model.

(a) Loading in RD.

(b) Loading in TD.

Figure 4: The macroscopic engineering stress-strain response of the RVE (solid black lines), compared to the data obtained from tensile experiments (coloured dots) from Shen et al. [25]. Loading is performed in both the rolling direction and transverse direction at different temperatures.

4. Cleavage criterion

Now that the material model parameters are identified, a criterion is needed that allows to identify the instant at which the material loses its load-bearing capacity. In order to demonstrate this, a tensile test is simulated using RVE A as described in section 3.1, with a strain rate of $\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$ in TD at a temperature $T = 265 \text{ }^\circ\text{C}$. The macroscopic response of such a tensile test is obtained as follows:

$$\bar{\sigma} = \frac{1}{\bar{J}} \bar{\mathbf{P}} \cdot \bar{\mathbf{F}}^T, \quad (24)$$

with $\bar{\mathbf{F}}$ the second-order macroscopic deformation gradient tensor and $\bar{J} = \det(\bar{\mathbf{F}})$. The first principal value of the macroscopic Cauchy stress $\bar{\sigma}$ is denoted as $\bar{\sigma}_1$. In figure 5a, $\bar{\sigma}_1$ is visualised as a function of the engineering strain by the solid line. In order to identify the instant of cleavage, one could adopt a Rankine-type of criterion, as used by for instance Needleman and Tvergaard [26] or Ritchie et al. [27]. In this criterion, cleavage occurs when the average of the local maximum principal stress exceeds some material dependent threshold within a certain region. Typically, the size of this region is comparable to the size of a grain. Since both the elastic modulus and surface energy do not change rapidly with temperature, the critical principal stress σ_c (the threshold value) is typically taken to be temperature and strain rate independent [28]. Furthermore, the critical principal stress is not dependent on strain rate because it is not based on plastic deformation. If for one of the grains this criterion is met, it is assumed that a crack will run through the material in an unstable manner. In each of the grains, the average stress σ_g^i in grain i is defined as

$$\sigma_g^i = \langle \sigma(\vec{x}) \rangle_{V_g^i} \quad (25)$$

The first principal value of the grain averaged stress σ_g^i is denoted as $\sigma_{g,1}^i$. In figure 5a, for each grain, the first principal value of the average stress and first principle value of the average strain at a macroscopic engineering strain of 2% is plotted as a black dot. If $\max(\sigma_{g,1}^i) = \sigma_c$ would be taken as the failure criterion, then only a single outlier (the ‘‘cleavage grain’’) of this point-cloud would dictate the moment of failure. The onset of failure would then strongly depend on the actual realization of the grain orientations. If the principle stresses follow a normal distribution, the moment of failure would never reach a steady solution as more grains are included. Hence, a different cleavage criterion is proposed, based on statistical measures of the grain-averaged first principal stress $\sigma_{g,1}^i$:

$$\langle \sigma_{g,1}^i \rangle = \frac{\sum_i V_g^i \sigma_{g,1}^i}{V_{\text{RVE}}}, \quad \text{sd}(\sigma_{g,1}^i) = \sqrt{\frac{\sum_i V_g^i (\sigma_{g,1}^i - \langle \sigma_{g,1}^i \rangle)^2}{V_{\text{RVE}} (N_g - 1) / N_g}}. \quad (26)$$

where $\langle \sigma_{g,1}^i \rangle$ is the mean value and $\text{sd}(\sigma_{g,1}^i)$ is the standard deviation, both weighted by the grain volumes. Note that in the case of a heterogeneous stress-field $\sigma(\vec{x})$, $\langle \sigma_{g,1}^i \rangle$ is slightly larger than the macroscopic first principal stress $\bar{\sigma}_1$ due to misalignment of the first principal stress directions in the different grains. This implies that the volume averaging operator and the first principal component are not permutable. In figure 5b, the distribution of the grain-averaged first principal stresses $\sigma_{g,1}^i$ from figure 5a is shown. As a reference, a normal probability density function is indicated by the solid line with the mean and standard deviation as indicated by equation (26). Note that the distribution of $\sigma_{g,1}^i$ follows a normal distribution rather closely. The alternative failure criterion here is based on the following equivalent cleavage stress

$$\hat{\sigma} = \langle \sigma_{g,1}^i \rangle + c_{\text{sd}} \text{sd}(\sigma_{g,1}^i), \quad (27)$$

with c_{sd} a constant larger than zero. Cleavage occurs when $\hat{\sigma}(\sigma_{g,1}^i) = \sigma_c$, which is a mean-field type of cleavage criterion.

If $\hat{\sigma}(\sigma_{g,1}^i) = \sigma_c$ is satisfied during loading and $c_{\text{sd}} = 2.33$ is taken, then statistically 1% of the grains has a stress above the critical value σ_c in case of a normal distribution. The value $c_{\text{sd}} = 2.33$ is adopted in the remainder of this work. The value of $\hat{\sigma}(\sigma_{g,1}^i)$ is visualised in figure 5b by the dashed line. Although this 1% threshold is still rather arbitrary, it is statistically much better defined.

In each loading direction (TD, ND and RD), tensile experiments are simulated. The simulations are performed at a strain rate of $\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$ and a temperature of $T = 250 \text{ }^\circ\text{C}$. The two cleavage

(a) The macroscopic response $\bar{\sigma}_1$ of a tensile test (solid line) and the grain-averaged stresses $\sigma_{g,1}^i$ (dots) at 2% macroscopic strain.

(b) Distribution of the first principal stresses $\sigma_{g,1}^i$ (bar plot), compared to a normal distribution (dashed line). The dashed line indicates the newly proposed cleavage criterion.

Figure 5: Statistics for the grain-averaged stresses $\sigma_{g,1}^i$ at 2% macroscopic strain. A strain rate of $\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$ is applied in TD, on an RVE consisting of 576 grains, at a temperature $T = 265 \text{ }^\circ\text{C}$.

criteria discussed above are compared next. In figure 6a, the maximum grain-averaged first-principal stress $\max(\sigma_{g,1}^i)$ is plotted as a function of macroscopic engineering strain. In this figure, the colors of the lines correspond to the RVE the simulation was performed on, as indicated in figure 3. Each simulation is performed five times with the same set of crystallographic orientations but each time assigned to different microstructural grains. This basically implies that the neighbours of grains are shuffled in each simulation. In figure 6b, the newly proposed criterion of equation (27) is shown as well as the mean and standard deviation of the grain-averaged stresses. The spread in the newly proposed equivalent cleavage stress is significantly less compared to the spread in the maximum value of the grain averaged first principle stress, even though the orientation distribution function is exactly the same. Accordingly, the newly proposed cleavage criterion is statistically better defined. Nevertheless, in the remainder of this paper, the instant of cleavage is obtained by averaging out this spread in equivalent stress $\hat{\sigma}$. For each loading condition, simulations are performed on the two RVEs for which it holds that the loading direction is perpendicular to the thickness direction of the RVE and with five microstructural realizations each (in which the neighbours of the grains are shuffled).

(a) Maximum grain-averaged first principal stress as a function of macroscopic engineering strain.

(b) Proposed equivalent cleavage stress as a function of macroscopic engineering strain, see equation (27).

Figure 6: Comparison of two cleavage criteria. Cleavage is assumed to occur when the local first principal stress averaged over a single grain reaches a (temperature and strain rate independent) critical value (a); or when the equivalent cleavage stress exceeds this critical value (b). The colors of the lines correspond to the RVE the simulation was performed on, as indicated in figure 3.

In figure 7a, the equivalent cleavage stress is shown as a function of the macroscopic engineering strain while loading in TD in the temperature range 240 – 280 °C. The intersections of these curves with the critical cleavage stress σ_c mark the instant at which fracture occurs. The critical value σ_c that corresponds to brittle failure is difficult to determine from experiments. The cleavage stress is generally strongly dependent on the presence of different kinds of impurities as well as on the grain size. Here $\sigma_c = 820$ MPa is taken, for which realistic results are obtained in terms of the brittle-to-ductile transition temperature and activation energy as will be shown in section 5. In figure 7b, the corresponding macroscopic stresses are shown. Here, fracture is indicated with an x-mark.

Note that in contrast to e.g. Soyarslan et al. [29], the energy dissipation associated with brittle damage nor the evolution of damage is included in the current modelling framework. With the approach presented, the instant of failure can be identified during post analysis, without changing material parameters or element removal during the crystal plasticity simulation itself. Therefore, no gradual strength and stiffness loss is modelled. Since only the onset of brittle failure is required to identify the brittle-to-ductile transition temperature, the evolution of damage is not required for the present analysis.

(a) Equivalent stress as a function of macroscopic eng. strain for different temperatures, see equation (27).

(b) Macroscopic stress as a function of macroscopic engineering strain for different temperatures.

Figure 7: Cleavage simulations performed in TD at a strain rate of $\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$. The X-marks indicate the onset of cleavage.

5. Brittle-to-ductile transition

At low temperatures, tungsten behaves rather brittle. Above the brittle-to-ductile transition temperature T_{bdt} , the behaviour tends to be more ductile. For modelling purposes, this transition needs to be properly defined. To this end, the following criterion is adopted:

$$\begin{cases} \text{Brittle behaviour:} & \epsilon_f < 1\% , \\ \text{Ductile behaviour:} & \text{otherwise} . \end{cases} \quad (28)$$

Here, ϵ_f is the macroscopic strain-to-failure in the tensile direction, i.e. the macroscopic engineering strain at which the equivalent cleavage stress $\hat{\sigma}$ equals the critical stress σ_c . In figure 8, the strain-to-failure is shown as a function of temperature at a strain rate of $\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$ while loading in RD. The temperature at which the engineering strain-to-failure equals 1% is identified as the brittle-to-ductile transition temperature, which is found to be $T_{\text{bdt}} = 249^\circ\text{C}$ for these loading conditions.

With the brittle-to-ductile transition being defined, loading directions TD, ND and RD can be compared. Due to the texture, the mean value of the stress $\langle \sigma_{g,1}^i \rangle$, and therefore the equivalent cleavage stress $\hat{\sigma}$ is highest when loading in ND, see figure 9. In the figure, the equivalent cleavage stress is compared to the critical stress σ_c , which is indicated by the (horizontal) dashed line. The engineering strain at which $\hat{\sigma} = \sigma_c$, is referred to as the strain-to-failure ϵ_f . From the figure it can be seen that under the same loading conditions, cleavage occurs at the lowest macroscopic strain when the specimen is loaded in ND. This suggests that the response in ND is most brittle.

Figure 8: Strain-to-failure as function of temperature for loading in RD at a strain rate of $\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$. The temperature at which the strain-to-failure equals 1% marks the brittle-to-ductile transition temperature.

Figure 9: The equivalent stress $\hat{\sigma}$, the grain average first principle stress $\langle \sigma_{g,1}^i \rangle$ and its standard deviation as function of macroscopic engineering strain for loading directions TD, ND and RD, at a fixed strain rate of $\dot{\epsilon} = 10^{-3} \text{ s}^{-1}$ and temperature of $T = 250 \text{ }^\circ\text{C}$.

(a) The strain-to-failure as function of temperature for different loading directions and strain rates.

(b) The brittle-to-ductile transition temperature as a function of strain rate for different loading directions.

Figure 10: A comparison between three loading directions (TD, ND and RD) in terms of strain-to-failure, brittle-to-ductile transition temperature and activation energy.

The strain-to-failure ϵ_f is plotted as a function of temperature T in figure 10a. With increasing strain rate, the transition temperature also increases while loading in TD, ND or RD. The transition temperature is plotted as function of the strain rate in figure 10b. As found in experiments by e.g. Giannattasio and Roberts [2], the brittle-to-ductile transition temperature T_{bdt} is dependent on the strain rate $\dot{\epsilon}$ following an Arrhenius-type of equation:

$$T_{\text{bdt}} = \frac{-E_{\text{bdt}}}{k_B \ln(\dot{\epsilon}/\dot{\epsilon}_0)}, \quad (29)$$

where E_{bdt} denotes the so-called brittle-to-ductile activation energy and k_B the Boltzmann constant. The pre-exponential factor $\dot{\epsilon}_0$ is a microstructure-specific constant, independent of temperature and strain rate. By fitting equation (29), the activation energy E_{bdt} can be obtained for different loading directions. In the current work, an activation energy of $E_{\text{bdt}} = 0.95 \text{ eV}$ is found in TD, while $E_{\text{bdt}} = 0.95 \text{ eV}$ is found in ND, and $E_{\text{bdt}} = 0.91 \text{ eV}$ is found in RD.

6. Discussion

Several parameters of the constitutive model have been identified from the experimental results of Shen et al. [25]. The corresponding samples had a grain size of approximately $330 \times 140 \times 40 \text{ } \mu\text{m}$ (in RD,

TD and ND respectively). However, no EBSD data is available for these samples. The texture used in the current work was obtained from commercial tungsten samples from AT&M, also produced by rolling. The grain size of these samples is roughly 96 μm , which is very similar to the samples from Shen et al. [25]. The ODF of the crystal orientations reveal a similar pattern as observed for unidirectionally rolled pure W by Zhang et al. [30]. However, the intensity of the preferred crystal orientations as adopted in the current work is significantly less pronounced. Note that the intensity of the crystallographic texture determines the anisotropy of the mechanical response as well as the anisotropy of the brittle-to-ductile transition temperature.

In the current work, the slip resistance consists of two parts; the kink-pair slip resistance and the hardening slip resistance. The kink-pair slip resistance governs the dislocation mobility at low temperatures as it is thermally activated, and it strongly decreases with increasing temperature. Since this is the (only) term that is temperature dependent, it here also controls the brittle-to-ductile transition temperature T_{bd}^{t} and the activation energy E_{bd}^{t} . This is in line with Giannattasio and Roberts [2], who argue that the processes controlling the T_{bd}^{t} is dislocation mobility.

Shen et al. [25] observed that the failure mode of their hot-rolled samples is transgranular cleavage both above and below the brittle-to-ductile transition temperature. In other papers in literature, also intergranular cleavage is reported [4]. In that case, the authors propose that a mixed criterion should be adopted where also the stress normal to the grain boundaries is compared to a critical value. Intergranular failure is not taken into account in the current work.

In order to investigate various aspects with respect to the brittle-to-ductile transition of high purity tungsten, Reiser et al. [5] performed Charpy impact tests on cold-rolled, hot-rolled and annealed high purity tungsten samples. The samples were unnotched high purity tungsten bars (dimension $1 \times 3 \times 27 \text{ mm}^3$). These bars were cut out in different orientations with respect to the rolling direction of the slab. The samples were cut in such a way that due the impact of the striker (in ND), bending occurred either along RD or TD. Reiser et al. [5] reported a strain rate of the outer fibres of 267.9 s^{-1} . The results of the experiments show that the brittle-to-ductile transition temperature of the sample loaded in RD is roughly 100 $^{\circ}\text{C}$ lower compared to a sample loaded in TD. This applied to both the hot-rolled and cold-rolled samples. In the current work, the brittle-to-ductile transition temperature is also found to be lower in RD compared to TD, which is in line with the results of Reiser et al. [5]. However, the difference is significantly smaller. The difference in T_{bd}^{t} is 16 $^{\circ}\text{C}$ at a strain rate of 10^{-3} s^{-1} , and is found to be dependent on the strain rate. The difference in T_{bd}^{t} increases with increasing strain rate. Therefore, the discrepancy may be due to the large difference in strain rate. Moreover, in the work of Reiser et al. [5], the texture and grain size may be significantly different compared to what was adopted in the current work.

The material parameters in the current work have been identified from the tensile data presented by Shen et al. [25], see figure 4a. They reported that the brittle-to-ductile transition is experimentally observed around 250 $^{\circ}\text{C}$ while loading in RD. Regarding loading in TD, Shen et al. [25] reported a brittle-to-ductile transition temperature around 300 $^{\circ}\text{C}$. The temperatures at which they performed their tensile tests were in the range of $150 < T < 500 \text{ }^{\circ}\text{C}$, with steps of 50 $^{\circ}\text{C}$. The difference in T_{bd}^{t} due to loading in RD compared to loading in TD may therefore be well smaller than 50 $^{\circ}\text{C}$. A difference in T_{bd}^{t} of 16 $^{\circ}\text{C}$, as obtained here, may therefore still be accurate.

In literature, the activation energy E_{bd}^{t} (describing the rate dependence of the T_{bd}^{t}) was experimentally determined in a number of papers. However, the obtained results from these studies seem to be rather far apart. For instance, Gmbsch et al. [6] found an activation energy of $E_{\text{bd}}^{\text{t}} \approx 0.2 \text{ eV}$ (on single crystal samples). In three other studies, an activation energy between 1.0-1.5 eV was found for different kinds of samples and loading conditions [2, 3, 7]. The latter results are rather close to what was found here. Nmeth et al. [4] reported an activation energy of $E_{\text{bd}}^{\text{t}} \approx 2.9 \text{ eV}$ (+2.6/-0.9 eV). They investigated the T_{bd}^{t} as a function of strain rate in the range of $\dot{\epsilon} = 3 \cdot 10^{-3} - 3 \cdot 10^{-6} \text{ s}^{-1}$. To this end, they performed a number of (unnotched) four-point-bending experiments. The grain size of their annealed high purity tungsten samples (grain size $d \approx 23 \mu\text{m}$) is significantly smaller than the grain size of the samples analysed in the current work. They showed that their T_{bd}^{t} increases with only about 10 $^{\circ}\text{C}$ when increasing the strain rate with one order of magnitude, which is less than the findings in the current work (52.5 $^{\circ}\text{C}$ in RD). The resulting activation energy was $E_{\text{bd}}^{\text{t}} = 2.9 \text{ eV}$ (+2.6/-0.9 eV), which is significantly higher than the results shown here ($E_{\text{bd}}^{\text{t}} = 0.91 \text{ eV}$ in RD). The origin of all these discrepancies is so far unclear. Giannattasio et al. [2] presented an overview of the activation energy as a function of the T_{bd}^{t} for a large collection of materials. They observed a clear trend, indicating that for

tungsten, the activation energy should be roughly 1.0 eV, which is in line with the results obtained in this paper.

7. Conclusions

In nuclear fusion reactors, the tungsten plasma facing components are subjected to extreme conditions, among which large (pulsating) heat flows. The tungsten components in fusion reactors should have their operating temperature above the brittle-to-ductile transition temperature in order to prevent brittle cleavage. To this end, a low transition temperature is more favourable as it increases the operating temperature range in which the response remains ductile.

The ductile behaviour of tungsten is governed by the motion of screw dislocations through the lattice and is described here with a crystal plasticity model. The rate of slip is modelled with a power law, which depends on the ratio between the resolved shear stress and the slip resistance. It can be concluded that with the crystal plasticity material model in the present work (along with the crystal orientations and the material parameters) the mechanical behaviour of high purity tungsten is adequately described at temperatures around the brittle-to-ductile transition temperature.

If a small fraction of the grains in a representative volume element is subjected to a first principal stress above a (strain rate and temperature independent) critical stress, the structure is prone to cleavage. This phenomenon is described by means of a new failure criterion which takes into account the mean value and standard deviation of the grain-averaged first principal stress. With this cleavage criterion, the onset of cleavage is statistically much better defined compared to a criterion based on the maximum principle stress, as used in literature. The temperature at which the engineering strain-to-failure is equal to a critical value, is marked as the brittle-to-ductile transition temperature T_{bd} . Here, $T_{\text{bd}} = 249$ °C was found by loading in the rolling direction, and a larger brittle-to-ductile transition temperature of $T_{\text{bd}} = 265$ °C was found for the transverse direction. The highest brittle-to-ductile transition temperature was found in the normal direction, with $T_{\text{bd}} = 268$ °C. The behaviour in this direction is therefore expected to be the most brittle.

Since the material model is rate dependent, the T_{bd} can be obtained at different strain rates. It is shown that the transition temperature increases with increasing strain rate. An activation energy of $E_{\text{bd}} = 0.91$ eV for this strain rate dependence was obtained by loading in the rolling direction and $E_{\text{bd}} = 0.95$ eV for the transverse direction and normal direction. These values are in line with experimental data in literature.

Also, it is shown that for rolled high-purity tungsten, the T_{bd} shifts to a higher temperature when the sample is loaded in its transverse direction instead of the rolling direction. This is also in line with experimental data. This difference in T_{bd} originates from the anisotropic texture of rolled tungsten.

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Author statement

Mathieu Oude Vrielink: Conceptualization, data curation, formal analysis, investigation, methodology, software, validation, visualization, writing – original draft.

Hans van Dommelen: conceptualization, funding acquisition, methodology, project administration, supervision, writing – review & editing.

Marc Geers: conceptualization, funding acquisition, methodology, resources, supervision, writing – review & editing.

Numerical investigation of the brittle-to-ductile transition temperature of rolled high-purity tungsten

M.A. Oude Vrielink, J.A.W. van Dommelen, M.G.D. Geers

Conflict of interest statement

This study and the manuscript present no conflict of interest.

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