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Computational analysis of the evolution of the brittle-to-ductile transition of tungsten under fusion conditions

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Abstract

Tungsten components inside fusion reactors are subjected to extreme conditions, including an exceptionally high heat flux. This loading induces high stress levels, that may lead to brittle fracture. The current work aims to provide novel insights by relating the risk for brittle fracture to the tungsten microstructure and loadings conditions. To this end, a crystal plasticity framework is adopted with a temperature dependent slip resistance. The required parameters are obtained from experimental data in the literature. The risk for brittle fracture is assessed by means of Beremin's weakest-link theory. The brittle-to-ductile transition temperature found in literature can be accurately described with the presented framework. The simulation results reveal that the brittle-to-ductile transition temperature decreases linearly with the volume fraction of recrystallized grains in the microstructure. It is also shown that a sharp interface between rolled and recrystallized microscopic grains is more favourable in terms of risk for brittle fracture.

Keywords: Crystal plasticity, tungsten, brittle-to-ductile transition, weakest-link theory

1. Introduction

Nuclear fusion has a great potential in meeting the future's increasing energy demand. It is a sophisticated technology that has a number of compelling advantages over more traditional methods, since it can provide power in a way that is intrinsically safe, practically limitless, environmental footprint free, and continuous over time.

In nuclear fusion reactors, the hydrogen isotopes tritium and deuterium are fused to form helium and a neutron. In order for this process to occur, an extraordinarily high temperature is required at which the particles behave as a plasma. The vast amount of energy that is released during the fusion process, results in a staggering heat flux of $10 - 20 \text{ MW/m}^2$ through the water-cooled plasma facing components of the reactor [1]. The large temperature gradient induced by these fluxes causes severe stresses in these components [2]. They should therefore be designed such that material failure is prevented.

Pure tungsten possesses a number of favourable properties that make it a compelling material for this application [3]. These include a high melting temperature, a high thermal conductivity, and a low sputtering yield [4]. Furthermore, tungsten behaves relatively ductile at elevated temperatures. However, the failure mechanism of tungsten at low temperature is brittle fracture, which occurs remarkably fast and is highly unwanted. Experiments indicate that the brittle-to-ductile transition temperature (BDTT) of tungsten is dependent on both the applied boundary conditions and the underlying microstructure [5-8].

The microstructure of the tungsten components under fusion conditions is evolving over time. The initial microstructure of the tungsten components investigated at present results from rolling, which was performed during the manufacturing process. This leads to a microstructure that consists of an aggregate of elongated grains with a preferred crystal orientation. As the tungsten component is subjected to high temperatures, the microstructure evolves due to recrystallization. In the reactor, this process occurs close

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to the plasma facing surface, where the initial microstructure is progressively replaced by nearly defect-free grains. The mechanical properties of these grains are different, since they have a lower resistance to plastic deformation compared to those in the original microstructure. Since the tungsten microstructure constantly evolves under fusion conditions, also the mechanical behaviour is evolving. This subsequently also influences the brittle-to-ductile transition temperature. In the current work, it is investigated how the brittle-to-ductile transition temperature of high-purity tungsten evolves under fusion conditions.

In the current work, the brittle-to-ductile transition temperature of tensile specimens is identified by assessing of the risk for brittle fracture at various temperatures. To this end, the weakest link theory is applied, as proposed by Beremin et al. [9], who introduced a probabilistic description of cleavage fracture. Here, the stressed region of a structure is divided into a number of sub-volumes. The probability of failure of the structure is assumed to equal the probability that failure occurs in any of these sub-volumes. Similar to Mathieu et al. [10], the stress state in these sub-volumes is assumed to be inhomogeneous. Instead, a multiscale approach is adopted where the microstructure is simulated by means of a representative volume element (RVE). The current work differs from the approach of Mathieu et al. [10] in the sense that here, the weakest link theory is applied on both the macroscopic and the microscopic scale.

After a review of the experimental observations in Sec. 2, a Laguerre-Voronoi diagram is adopted to closely mimic the observed microstructure in terms of grain size and texture in Sec. 3. For the resulting computational microstructure, the neighbours of each microscopic grain are the same as in the experimental observations. The mechanical behaviour of the grains is described in Sec. 4 by means of a crystal plasticity model with a temperature dependent slip resistance. The required material parameters are obtained from experimental data in literature. In order to assess the risk for brittle fracture in the tungsten specimen, Beremin's weakest-link theory is adopted in Sec. 5. This framework is applied to (partially-) recrystallized microstructures in Sec. 6, and subsequently also allows to relate the microstructure and loading conditions to the brittle-to-ductile transition temperature. Finally, in Sec. 7, the main findings and limitations of the current work are discussed.

2. Experimental observations

The heat generated by the fusion process is extracted in the divertor of the fusion reactor. This component contains CuCrZr cooling tubes which enable a continuous flow of water. A segment of such a cooling tube is visualized in Fig. 1 in orange. The cooling tubes are protected from the extreme conditions by means of tungsten monoblocks, as visualised in gray. The influence of high heat loads on the evolution of the microstructure of commercial tungsten monoblocks manufactured by AT&M, China, has been investigated by Shah et al. (2020) [11]. The monoblocks have dimensions of $28 \times 28 \times 12$ mm, and have an armour thickness of 8 mm. The production process of these monoblocks includes sintering, followed by hot rolling. The monoblock and the cooling tube are separated by a copper interlayer, as visualized in yellow in Fig. 1.

Fig. 1 shows the orthogonal coordinate system adopted at present. The grains have an aspect ratio of approximately 1:2, where the grains are elongated parallel to the direction in which the heat flux is applied. This direction is referred to as the height direction (HD) of the monoblock. The direction of the water flow (in the copper tube) is referred to as the tube direction (TD). Finally, the width direction (WD) of the monoblock is normal to both HD and TD.

The monoblocks were exposed to a high heat flux at the plasma facing surface, indicated by the wavering red arrows. The heat load follows the ITER qualification program and was applied by means of an electron beam at the IDTF in St. Petersburg, Russia. It consisted of 5000 cycles of 10 MW/m^2 and 1000 cycles of 20 MW/m^2 . Here, each cycle consisted of 10 seconds exposure time, followed by 10 seconds of dwelling. After the heat exposure, a specimen was extracted at 5 mm from the side of the monoblock by means of electrical discharge machining, as visualized in Fig. 1. This allowed for closer inspection of the TD-HD plane by means of EBSD analysis.

Due to the heat load, recrystallization occurred at the top region of the monoblock, generating new grains that are nearly defect free. The recrystallized grains consist of only few subgrains, characterized by low angle grain boundaries. The EBSD scan performed by [11] on the specimen shows the transition region between the initial microstructure and the recrystallized microstructure. From the EBSD scan, grain boundaries are identified by taking a threshold misorientation angle of 10 degrees. The grain

Figure 1: Heat exposed monoblock, from Shah et al. (2020) [11]. The EBSD colors indicate the crystal orientation in TD.

boundaries are indicated in the figure with black lines. The grain size distributions of the initial and recrystallized part of the specimen are approximately the same. This will be further highlighted in Sec. 3.

3. Representative volume element

In the current section, the rolled part (i.e. the bottom half) of the EBSD scan in Fig. 1 is investigated. The area of this part of the scan is $1000 \times 1000 \mu\text{m}^2$. In order to investigate the mechanical behaviour that corresponds to this microstructure, a periodic representative volume element (RVE) is generated from this EBSD scan.

The RVE is generated in four steps. First, the grains are assigned their respective mean crystal orientation in Fig. 2a. In this figure, the colors indicate the crystal orientations in TD, corresponding to the legend. Additionally, the centroids of each of the grains are identified and indicated with a black +. The area-weighted mean grain size equals $93 \mu\text{m}$. From the 250 largest grains identified, the centroids are taken as the initial guess for an algorithm that redistributes these coordinates such that the spacing between them is proportional to their grain size. This is shown in Fig. 2b, where the dashed square corresponds to the scanning area of $1000 \times 1000 \mu\text{m}^2$. Around each of the centroids, a sphere is drawn with an area equal to that of the corresponding grain. The spheres are copied periodically to the area surrounding the RVE in order to account for periodicity. In the algorithm adopted here, spheres that overlap repel each other. Therefore, the overlapping area is minimized, as shown in Fig. 2c. The algorithm ensures that the spacing between the centroids adequately matches the area of the corresponding grain, which makes it suitable for a Voronoi algorithm while preserving the grain size distribution. This is in line with the dynamic microstructure generator (DMG) used in [12]. Finally, a Laguerre-Voronoi algorithm is applied [13] where the radius of each of the spheres is entered as a weighing factor. The resulting cells are considered to be the grains of the RVE, as shown in Fig. 2(d).

A pronounced similarity can be observed between the generated RVE in Fig. 2d and the EBSD-scan in Fig. 2a. Note that the most dominant aspect of the microstructure for the mechanical response is the texture, whereas the effect of the aspect ratio on the grains is minimal. Hence, the latter effect is not

Figure 2: Step-by-step illustration of the RVE generation algorithm of the rolled microstructure. For each of these figures, the horizontal direction corresponds to TD, while the vertical direction corresponds to HD. The first figure shows the legend, where the colors indicate the crystal orientation in TD.

taken into account. Since the centroids of the grains are taken as initial guess for the dynamic model, grains generally preserve the same neighbours, which is expected to enhance the predictive capability of the model. The cumulative grain size distribution of the RVE is compared to the one from the EBSD scan for either rolled or recrystallized material, as shown in Fig. 3. The figure shows that although the smallest grains in the EBSD-scan are not included in the RVE, the overall grain size distribution in the RVE is in excellent agreement with the grain size distribution in the EBSD scan. Furthermore, the grain size distribution of the recrystallized part (i.e. the top half) of the EBSD scan in Fig. 1 is very similar to the grain size distribution of the rolled part (i.e. the bottom half). The mean grain area A_{mean} is calculated, whereby the area fractions of the grains are taken as weight factors. The mean grain area in the rolled part of the EBSD scan is $14.1 \cdot 10^3 \mu\text{m}^2$, which is similar to the mean grain area in the recrystallized part of the EBSD scan with $12.0 \cdot 10^3 \mu\text{m}^2$ and the mean grain area in the RVE, which equals $13.9 \cdot 10^3 \mu\text{m}^2$. The thickness b of the RVE is taken to be the square root of the mean grain area in the RVE, so $b = 118 \mu\text{m}$. This is required for computing the grain size as will be shown in Sec. 5.

From the area of the EBSD scan presented in Fig. 1 and indicated with 'rolled' (i.e. the bottom part), the orientation distribution function (ODF) in Fig. 4a is obtained. The colorbar shows the intensity of the crystal orientation, which is overall weak. However, regarding the (111) crystal orientation, there is a small preferred orientation in TD. The ODF obtained from the area of the EBSD scan indicated with 'recrystallized' is presented in Fig. 4b. The overall trends of the ODF obtained from these areas are clearly similar. In the representative volume element, each of the grains is assigned the mean orientation of the corresponding grain in the rolled part of the EBSD-scan, as shown in Fig. 4c. This induces a minor increase in the intensity of the crystal orientations in the ODF. However, the overall trends are well captured.

Figure 3: Grain size distribution: comparison between the RVE, the rolled part of the EBSD scan, and the recrystallized part of the EBSD scan.

The geometry shown in Fig. 4c is discretized into a single layer of 7934 (quadratic) serendipity brick-elements with reduced integration (8 integration points). This mesh is subjected to 3D periodic boundary conditions, in which the displacements of nodes on opposite surfaces are tied such that the structure also remains periodic during deformation. In thickness direction (i.e. WD), the top and bottom surface are also tied to each other. This is in line with Boeff [12], who also applied 3D periodic boundary conditions on an RVE with non-straight boundaries. Finally, uniaxial loading is applied in order to simulate a tensile test. The loading conditions are implemented such that an arbitrary loading direction can be prescribed, as described by Van Nuland et al. [14]. Here, the bottom-left corner node is fixed, while the displacement of the bottom-right corner node is coupled to the displacement of the top-left corner node such that the RVE remains macroscopically stress-free in any direction perpendicular to the loading direction.

4. Material model

In order to describe the material behaviour at a microscopic material point in the RVE, a finite strain crystal plasticity framework is adopted in a similar manner as presented by Asaro [15]. Within this framework, the plastic deformation is governed by slip on a pre-specified set of slip systems. The rate of slip on each of the slip systems is dependent on the ratio between the resolved shear stress and the resistance to slip. Since tungsten has a body centred cubic stacking of atoms, the model includes a slip resistance that strongly increases with decreasing temperature.

4.1. Kinematics

The deformation gradient tensor $\mathbf{F}$ maps an initial position vector to the deformed configuration. It consists of an elastic part $\mathbf{F}_e$ 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 as follows

$$\mathbf{L}_p = \dot{\mathbf{F}}_p \cdot \mathbf{F}_p^{-1} = \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{P}_0^{\alpha} = \sum_{\alpha} \dot{\gamma}^{\alpha} \bar{\mathbf{s}}_0^{\alpha} \bar{\mathbf{n}}_0^{\alpha} . \quad (2)$$

Here, $\dot{\gamma}^{\alpha}$ is the slip rate on slip system $\alpha = 1, 2, \dots, N_s$ with N_s the number of slip systems. The Schmid tensor $\mathbf{P}_0^{\alpha}$ is composed of the diadic product of the slip direction $\bar{\mathbf{s}}_0^{\alpha}$ and the slip plane normal $\bar{\mathbf{n}}_0^{\alpha}$ in the undeformed configuration. In the current work, only the $\{\bar{1}01\} \langle 111 \rangle$ family of slip systems is assumed to be active [16–18], hence $N_s = 12$.

Figure 4: Equal area projections (upper hemisphere) of the orientation distribution function (ODF). The texture of the recrystallized part follows the same trends as the rolled part of the EBSD scan. In the RVE, each cell is assigned the average crystal orientation of the grain it corresponds to, causing a minor increase in the ODF intensity.

4.2. Elastic contribution

The elastic response is described by means of the second-order second Piola-Kirchhoff stress tensor in the intermediate configuration $\mathbf{S}_e$, which is calculated as

$$\mathbf{S}_e = \mathbf{F}_p \cdot \mathbf{S} \cdot \mathbf{F}_p^T = {}^4\mathbb{C} : \mathbf{E}_e . \quad (3)$$

Here, $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor and ${}^4\mathbb{C}$ is the fourth-order elasticity tensor. The elastic response is assumed to be isotropic, composed of bulk modulus κ and shear modulus G . Furthermore, the second-order Green-Lagrange strain tensor $\mathbf{E}_e$ is defined as

$$\mathbf{E}_e = \frac{1}{2} (\mathbf{C}_e - \mathbf{I}) , \quad (4)$$

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

4.3. Crystallographic slip

Plasticity is accommodated by the nucleation and propagation of dislocations through the tungsten lattice, inducing slip on slip systems. In the current work, the slip rate is described by means of a power-law, which implies that a rate dependent flow rule is adopted:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{|\tau^\alpha|}{s^\alpha} \right)^{1/m} \text{sign}(\tau^\alpha) . \quad (5)$$

Here, the material parameter $\dot{\gamma}_0$ is the reference slip rate, and the parameter m is the strain rate sensitivity. The rate of slip is dependent on the ratio between the resolved shear stress τ^α and the resistance to slip s^α . The resolved shear stress on slip system α is given as

$$\tau^\alpha = \mathbf{S}_e \cdot \mathbf{C}_e : \mathbf{P}_0^\alpha . \quad (6)$$

The slip resistance s^α on slip system α is additively split into two contributions as follows

$$s^\alpha = s_{\text{obs}}^\alpha + s_{\text{kp}}^\alpha , \quad (7)$$

where the obstacle slip resistance s_{obs}^α is the temperature independent part that increases with the amount of accumulated slip and the kink-pair slip resistance s_{kp}^α is the thermally activated contribution that increases with decreasing temperature.

4.3.1. Obstacle slip resistance

Dislocations multiply with an increasing amount of slip. Dislocation lines subsequently entangle and obstruct one another, causing the resistance to slip to increase. The time derivative of this type of slip resistance is phenomenologically described and given by

$$\dot{s}_{\text{obs}}^\alpha = \sum_{\beta} h^{\alpha\beta} |\dot{\gamma}^\beta| , \quad (8)$$

where $h^{\alpha\beta}$ is the hardening matrix, given by

$$h^{\alpha\beta} = q^{\alpha\beta} h_0 \left(1 - \frac{s_{\text{obs}}^\beta}{s_\infty} \right)^a . \quad (9)$$

Here, the hardening exponent a , saturation slip resistance s_∞ and initial hardening rate h_0 are material parameters. For self-hardening it holds that $q^{\alpha\alpha} = 1$, while the terms $\alpha \neq \beta$ represent latent-hardening for which $q^{\alpha\beta} = q_n$. The obstacle slip resistance on each of the slip systems monotonically increases with the amount of slip from the initial slip resistance $s_{\text{obs},0}$ to the saturation slip resistance s_∞ .

4.3.2. Kink-pair slip resistance

Dislocations must overcome the periodic resistance of the crystal lattice in order to propagate through the material. This type of barrier, also referred to as the Peierls barrier, is thermally activated and negligibly low at elevated temperatures. Dislocation lines overcome these barriers by the formation of kink-pairs. The slip resistance that follows is formulated as

$$s_{\text{kp}}^\alpha = s_{\text{kp},0} \left[1 - \left(\frac{T}{T_k^\alpha} \right)^{\frac{1}{q}} \right]^{\frac{1}{p}} , \quad (10)$$

with exponents $0 \leq p \leq 1$ and $1 \leq q \leq 2$ and $s_{\text{kp},0}$ the kink-pair slip resistance at $T = 0$ K. The shear-rate dependent knee temperature T_k^α of slip system α is taken as proposed by Lim et al. [19], but is slightly modified with $\dot{\gamma}_{\text{corr}}$ in order to make Eq. (10) a smooth function of $\dot{\gamma}^\alpha$:

$$T_k^\alpha = \frac{-G_0}{k_b \ln((|\dot{\gamma}^\alpha| + \dot{\gamma}_{\text{corr}})/\dot{\gamma}_{\text{kp},0})} , \quad (11)$$

with G_0 the activation energy, k_b the Boltzmann constant, $\dot{\gamma}_{\text{kp},0}$ the reference kink-pair rate. Note that no solution exists for s_{kp}^α if $T_k^\alpha > T$. However, since the correction $\dot{\gamma}_{\text{corr}}$ is taken to be

$$\dot{\gamma}_{\text{corr}} = \dot{\gamma}_{\text{kp},0} \left[\exp \left(\frac{-G_0}{T k_b} \right) + \epsilon \right] , \quad (12)$$

this anomaly is circumvented. Furthermore, $\epsilon = 10^{-8}$ is an arbitrary small value that ensures that s_{kp}^α is no longer over sensitive to low values of $\dot{\gamma}^\alpha < \epsilon$.

4.4. Material characterization

The parameters of the above material model based on crystal plasticity have been identified for the rolled (initial) microstructure by Oude Vrielink et al. [20]. Most of the material parameters are assumed to remain unchanged as the material recrystallizes, as will be shown in section 4.4.1. However, the initial obstacle slip resistance and initial hardening rate reduce significantly due to the pronounced decrease in defect density in the recrystallized material as shown in section 4.4.2.

4.4.1. Material parameters from literature

Since no complete set of material parameters is available in literature, the material parameters in the current work are adopted from a variety of references. The parameters presented here are validated in Sec. 4.4.2. Regarding the slip law, the strain-rate sensitivity parameter m is taken from Asaro [15]:

$$m = 0.02 . \quad (13)$$

Later, Wei en Kecskes [21] found comparable outcomes of their strain-rate sensitivity experiments on different specimens for different rolling conditions. It is unknown how recrystallization influences the strain-rate sensitivity parameter for tungsten. In this work, it is therefore assumed to remain unchanged. Regarding the kink-pair slip resistance, several parameters are required. The activation energy is adopted from Brunner [22]:

$$G_0 = 1.75 \text{ eV} . \quad (14)$$

Furthermore, the exponents p and q are taken such that the resulting potential closely approximates the Eshelby potential [23]:

$$p = 0.8 , \quad q = 1.2 . \quad (15)$$

The reference kink-pair slip rate is taken from Lim et al. [19], who identified this parameter from the single-crystal data from Brunner [22]:

$$\dot{\gamma}_{\text{kp},0} = 3.71 \cdot 10^{10} \text{ s}^{-1} . \quad (16)$$

The parameters required to construct the isotropic elasticity tensor ${}^4\mathbb{C}$ are taken from Lowrie and Gonas [24], while neglecting their temperature dependency:

$$\kappa = 309 \text{ GPa} , \quad G = 161 \text{ GPa} . \quad (17)$$

The hardening parameters that are required for the expression of the obstacle slip resistance include the hardening exponent a that is taken from Yalçinkaya et al. [25]. The hardening matrix coefficients are taken from Asaro [15]:

$$a = 1.5 , \quad q_n = 1.4 . \quad (18)$$

Finally, the reference slip rate parameter $\dot{\gamma}_0$, the saturation slip resistance s_∞ and the kink-pair slip resistance extrapolated to $T = 0 \text{ K}$ are adopted from Oude Vrielink et al. [20]:

$$\dot{\gamma}_0 = 10^{-3} \text{ s}^{-1} , \quad s_\infty = 210 \text{ MPa} , \quad s_{\text{kp},0} = 600 \text{ MPa} . \quad (19)$$

4.4.2. Material parameters from experimental data

Regarding the recrystallized material, the remaining parameters are identified from the experimental data of Younger and Wrights [26]. To this end, crystal plasticity simulations are performed with prescribed displacements at a strain-rate of $\dot{\epsilon} = 3.35 \cdot 10^{-3} \text{ s}^{-1}$ in order to match the tensile experiments of Younger and Wrights [26]. From the simulation results, the macroscopic stress is obtained in terms of the first Piola-Kirchhoff stress by taking its volume average over the entire RVE:

$$\bar{\mathbf{P}} = \frac{1}{V_{\text{RVE}}} \int_{V_{\text{RVE}}} \mathbf{P}(\vec{x}) \text{ d}V . \quad (20)$$

In order to demonstrate the macroscopic behaviour of the material model, a finite element simulation is performed on a simple RVE that consists of a grid of $24 \times 24 \times 1$ randomly oriented grains, discretized by $72 \times 72 \times 1$ quadratic brick elements with reduced integration, as shown earlier in Oude Vrielink et al. [20]. The RVE is subjected to 3D periodic boundary conditions and uniaxial loading. The blue solid line in Fig. 5a shows the engineering stress as a function of the plastic strain up to 15% at a temperature of $T = 867$ K, at which the response is nearly temperature independent. In order to obtain this result, the initial obstacle slip resistance $s_{\text{obs},0}$ is taken to be:

$$s_{\text{obs},0} = 40 \text{ MPa} . \quad (21)$$

Furthermore, the initial hardening rate h_0 is taken to be:

$$h_0 = 350 \text{ MPa} . \quad (22)$$

The dashed blue line shows the experimental results from Younger and Wrights [26] for comparison. Sheng et al. [27] obtained comparable results from their tensile tests on recrystallized tungsten specimens at 773 K. The parameters of rolled tungsten are taken identical as for recrystallized tungsten, except for the initial obstacle slip resistance $s_{\text{obs},0} = 170$ MPa and the initial hardening rate $h_0 = 3$ GPa [20]. In Fig. 5a, the comparison is shown between the crystal plasticity simulations and the tensile data from Shen et al. [28] in the regime where necking is negligible. The texture for this simulation is also taken from Oude Vrielink et al. [20].

(a) Comparison of hardening behaviour between the simulation results (CP) and the experimental data at the respective temperatures.

(b) Comparison between the simulation results (CP) and the experimental data of the temperature dependent yield stress of rolled and recrystallized tungsten. The light blue dots represent the brittle fracture strength.

Figure 5: The mechanical behaviour of tungsten in the rolled and recrystallized state compared to the experimental results from Younger and Wrights [26] and Shen et al. [28].

In figure 5b, the yield stress is plotted in the temperature range $400 \leq T \leq 1200$ K. Here, the solid lines show the numerically obtained yield stress by taking the first Piola-Kirchhoff stress in the loading direction at 0.2% plastic strain offset. The red dots show the experimental data from Younger and Wrights [26] and Shen et al. [28]. Clearly, the macroscopic yield stress behaviour is well described by the model for both rolled and recrystallized tungsten.

5. Cleavage fracture modelling

For tungsten, there is a transition from brittle behaviour to ductile behaviour with increasing temperature. The current work aims to identify how this brittle-to-ductile transition temperature is dependent on the microstructure and boundary conditions. In contrast to ductile failure, for brittle cleavage, failure occurs abruptly. Here, the focus is on the onset of this brittle failure process. The extent to which a specimen is brittle is assessed by its probability of brittle failure. The probability of failure of a specimen

is derived from the stress field that is computed by means of the crystal plasticity model in conjunction with a representative volume element of the microscopic scale. Since cleavage is most frequently observed on one of the $\{100\}$ planes [29], this aspect is taken into account. Finally, the cleavage fracture model provides the probability of failure of both the microstructural RVE and the macroscopic specimen, allowing to compare results to experimental data.

5.1. Weakest link theory

A given specimen with volume V_{sp} is divided into N equi-sized subvolumes V_{sub}^i , where $i = 1, 2, \dots, N$. Beremin's [9] weakest-link theory states that a specimen will fail in an unstable manner if failure occurs in one of the volumes V_{sub}^i . The probability of failure of the specimen $P_{\text{f,sp}}$ is therefore given by

$$P_{\text{f,sp}} = 1 - \prod_{i=1}^N [1 - p_{\text{f,sub}}^i] , \quad (23)$$

where $p_{\text{f,sub}}^i$ is the failure probability of a subvolume V_{sub}^i , which is governed by an equivalent stress state $\hat{\sigma}_i$ present in this volume. Eq. (23) can be simplified to

$$P_{\text{f,sp}} \approx 1 - \exp \left(- \sum_{i=1}^N p_{\text{f,sub}}^i \right) , \quad (24)$$

when $p_{\text{f,sub}}^i$ is small. In a tensile test, the failure probability can be regarded as homogeneous if the macroscopic stress field is homogeneous and the microstructure is not varying over the gauge section. In that case, all subvolumes have the same failure probability $p_{\text{f,sub}}$. The specimen failure probability is then given by:

$$P_{\text{f,sp}} = 1 - \exp \left(- \frac{p_{\text{f,sub}}}{V_{\text{sub}}} V_{\text{sp}} \right) . \quad (25)$$

Eq. (25) is visualized in Fig. 6, revealing that the combination of a large specimen volume V_{sp} with a high concentration of failure probability yields a high specimen failure probability $P_{\text{f,sp}}$.

Figure 6: Specimen failure probability as a function of specific local failure probability and specimen volume.

The approach of Beremin et al. [9] yields an adequate prediction of the probability of failure of a specimen. However, this model does not include any relation to the microstructure by means of a representative volume element. Also, it does not take into account the orientation of the cleavage planes. Therefore, in the current work, their model is extended such that it includes these aspects.

5.2. Flawed material

In order to include the influence of grain topology and crystal orientation, the ratio $p_{\text{f,sub}}/V_{\text{sub}}$ in Eq. (25) is replaced by $p_{\text{f,rve}}/V_{\text{rve}}$. Here, $p_{\text{f,rve}}$ is the failure probability of a representative volume element (RVE) with volume V_{rve} . The failure probability of the RVE is subsequently given by the probability

that one of the M grains fails. In other words, the weakest link theory is applied once more, but now at the microscopic scale:

$$p_{f,\text{rve}} = 1 - \prod_{j=1}^M (1 - p_{f,g}^j) , \quad (26)$$

where $p_{f,g}^j$ is the failure probability of grain j with volume V_g^j . Since both $p_{f,g}^j$ and the probability of failure of the RVE $p_{f,\text{rve}}$ are small, this equation can be simplified as follows:

$$p_{f,\text{rve}} = \sum_{j=1}^M p_{f,g}^j . \quad (27)$$

Grains are typically flawed due to material defects. These defects include microcracks that may have initiated during plastic deformation, for instance during the specimen manufacturing process. The probability of finding a micro-crack of a length between r and $r + dr$ in a reference volume V_{ref} is described by a power law [9]:

$$G(r) dr = \frac{\alpha}{r^\beta} dr . \quad (28)$$

In the current work, the reference volume V_{ref} is taken equal to the mean grain volume. The failure probability $p_{f,g}^j$ of a grain with volume V_g^j is governed by the probability of finding a micro-crack in this volume exceeding a critical crack length r_c . It can therefore be calculated by:

$$p_{f,g}^j = \frac{V_g^j}{V_{\text{ref}}} \int_{r_c}^{\infty} \frac{\alpha}{r^\beta} dr = \frac{V_g^j}{V_{\text{ref}}} \frac{\alpha}{\beta - 1} \left(\frac{1}{r_c} \right)^{\beta-1} , \quad (29)$$

where α and β are material parameters. According to Griffith's energy balance [30], the critical crack length is given by $r_c = (k_{\text{Griff}} / \langle \sigma_n \rangle)^2$, where k_{Griff} depends on the boundary conditions, the shape of the defect, the surface energy and the Young's modulus. The latter two are mildly dependent on temperature, but this aspect is neglected in the current analysis. A positive stress normal to the crack opening $\langle \sigma_n \rangle$ is indicated by Macaulay brackets:

$$\langle \sigma_n \rangle = \begin{cases} 0, & \sigma_n < 0 \\ \sigma_n, & \sigma_n \geq 0 \end{cases} \quad (30)$$

This expression can be substituted in Eq. (29), which can subsequently be rewritten into the following form:

$$p_{f,g}^j = p_0 \left(\frac{\langle \sigma_n \rangle}{\sigma_{\text{ref}}} \right)^{m_f} \frac{V_g^j}{V_{\text{ref}}} , \quad (31)$$

with material parameters p_0 , σ_{ref} and $m_f = 2\beta - 2$. In tungsten, cracks are mostly observed on the three cleavage planes $\{100\}$ [29] with normals $\vec{n}_{\text{cl}}^l$ where $l = 1, 2, 3$. A grain will fail if failure occurs on one of these planes. Assuming an equal micro crack distribution on these planes, Eq. (31) can be rewritten as

$$p_{f,g}^j = 1 - \prod_{l=1}^3 \left\{ 1 - p_0 \left(\frac{\langle \sigma_n^l \rangle}{\sigma_{\text{ref}}} \right)^{m_f} \frac{V_g^j}{V_{\text{ref}}} \right\} \approx \sum_{l=1}^3 p_0 \left(\frac{\langle \sigma_n^l \rangle}{\sigma_{\text{ref}}} \right)^{m_f} \frac{V_g^j}{V_{\text{ref}}} , \quad (32)$$

in which the approximation holds because $p_{f,g}^j$ is small. Since a specimen typically consists of many grains, the failure probability of a single grain is small, even when cleavage of the specimen is almost certain. However, in the limit case where the exponent m_f is large, the probability in Eq. (31) becomes a Heaviside function. Here, a grain will fail if a critical fracture stress equal to σ_{ref} is reached. If the specimen consists of only a single crystal, this reduces to the competition between the athermal strength and the temperature-dependent slip resistance. Note also that in this case, the simplifications made in Eq. (24) and Eq. (32) do not hold.

The Cauchy stress normal to the cleavage planes is given by

$$\sigma_n^l = \vec{n}_{cl}^l \cdot \boldsymbol{\sigma}_g \cdot \vec{n}_{cl}^l \quad \text{and} \quad \boldsymbol{\sigma}_g = \frac{1}{V_g} \int_{V_g} \boldsymbol{\sigma}(\vec{x}) dV \quad (33)$$

Substituting Eq. (32) into Eq. (27) allows for calculating the failure probability of the RVE. With this, the risk for brittle failure of the specimen can be assessed by means of Eq. (25) for a given microstructure and set of boundary conditions.

6. Results

The presented framework allows to compute the probability of brittle fracture. To this end, the RVE geometry presented in Sec. 3 is exploited, and combined with the material model and model parameters presented in Sec. 4. The risk for brittle fracture is assessed by means of the framework presented in Sec. 5. In the current work, the exponent m_f in Eq. (31) is taken from Margetson and Sherwood [31] and set to $m_f = 5.5$. Furthermore, the reference volume is set equal to the mean grain volume $V_{ref} = 1.64 \cdot 10^6 \mu m^3$. Parameter p_0 is set to $p_0 = 0.01$, such that if a grain with volume V_{ref} is subjected to an equivalent stress of σ_{ref} , its failure probability equals 1%. Parameter $\sigma_{ref} = 920$ MPa is taken, as this is found to provide realistic results for both rolled and recrystallized tungsten as will be shown in the remainder of this section. This implies that after recrystallization, the largest microscopic cracks that dictate the instant of failure remained unchanged in terms of size and density.

6.1. Validation

A tensile test of rolled tungsten is simulated up to 1% strain in vertical direction (HD) at a temperature of $T = 550$ K, using the RVE shown in Fig. 2d. The stresses are calculated using the crystal plasticity model in combination with the material parameters for rolled tungsten, and are shown in Fig. 7a. The resulting stress field σ_{22} is strongly heterogeneous, because each grain has a different crystallographic orientation. The average Cauchy stress in each grain in Fig. 8 is projected on its cleavage plane normals. From here, the failure probability of each grain can be computed with Eq. (32). In Fig. 7b, the failure probability is scaled by the grain size. Note that a large average stress in a grain does not necessarily result in a high probability of failure.

Figure 7: Results for a numerical tensile test on rolled tungsten at 1% strain and a temperature of $T = 550$ K.

The probability of failure is governed by the positive grain-averaged normal stress acting on the $\{100\}$ family of planes. In Fig. 8, these stress measures are plotted. In this figure, the location of each dot shows the orientation of the normal vector of one of the $\{100\}$ cleavage planes of each grain, while the color represents the normal stress acting on these planes. Only the upper hemisphere is shown, so for each grain three dots are plotted. The grain highlighted in green in Fig. 7 is also highlighted in Fig. 8. This grain shows that although its stress level is relatively low, it still has a high probability of failure due to the fact that it has a $\{100\}$ cleavage plane normal oriented parallel to the loading direction. Another grain, highlighted in purple in Fig. 7 and Fig. 8, shows exactly the opposite. Although its stress level is

relatively high, it has a low probability of failure since none of its cleavage plane normals are oriented close to the loading direction.

Figure 8: Relation between crystal orientation and the normal stress acting on the $\{100\}$ cleavage planes.

The same tensile test is now simulated at various temperatures and up to 2% strain. The specimen probability of failure is computed as a function of strain and temperature, see Fig. 9a. Here, a specimen volume $V_{sp} = 5 \times 1.5 \times 0.75 \text{ mm}^3$ is taken, in correspondence to the tensile experiments of Shen et al. (2016) [28]. The solid black lines in Fig. 9a indicate the probability curves of 10%, 50% and 90%. Clearly, with increasing strain and decreasing temperature, the risk for brittle fracture increases.

(a) Rolled tungsten, uniaxial loading on a specimen with a volume of $V = 5.6 \text{ mm}^3$.

(b) Recrystallized tungsten, uniaxial loading on a specimen with a volume of $V = 465.4 \text{ mm}^3$.

Figure 9: Failure probability of (a) rolled tungsten and (b) recrystallized tungsten in the temperature range of $350 \leq T \leq 550 \text{ K}$.

In the work of Shen et al. (2016) [28], a significant increase of the total elongation with increasing temperature was observed between 250 °C and 300 °C onwards. Shen et al. (2016) [28] therefore concluded that the brittle to ductile transition temperature must be in this range. From Fig. 9a it can be concluded that the brittle-to-ductile transition temperature depends on its actual definition. In the current work, the brittle-to-ductile transition temperature corresponds to the temperature at which the failure probability equals 50% at 1% of tensile strain. With this criterion, a transition temperature of $T_{bdt} = 261.1 \text{ °C}$ results. Therefore, in terms of brittle-to-ductile transition temperature, the numerical and experimental results are in close agreement.

Tensile experiments on recrystallized tungsten were performed by Younger and Wrights (1970) [26]. In their work, a clear increase in total elongation can be observed for $T \geq 550 \text{ K}$. The test specimens have $V_{sp} = 465.4 \text{ mm}^3$, which is significantly larger than those used by Shen et al. (2016) [28]. The numerical results corresponding to their specimen volume are shown in Fig. 9b and a brittle-to-ductile transition temperature of $T_{bdt} = 530.9 \text{ K} = 257.9 \text{ °C}$ is obtained. Again, an adequate agreement is found with the experimental results.

6.2. Partially recrystallized tungsten

The tungsten monoblocks initially possess a typical rolled microstructure. However, when the monoblocks are in operation, they are subjected to a high temperature. This causes recrystallization, in which new grains are formed with a low dislocation density. Due to this low defect density, these grains have different material properties. In this section, it is investigated how the brittle-to-ductile transition temperature of tungsten evolves under fusion conditions, during which the originally rolled microstructure recrystallizes.

All of the 250 grains in the initial microstructure are assumed to have the material properties of rolled tungsten, as shown by the blue grains in Fig. 10a. In order to simulate the mechanical behaviour of partially recrystallized tungsten, 50 grains are randomly selected and assigned the material properties of recrystallized tungsten in Fig. 10b. In this figure, the recrystallized grains are highlighted in red. In Fig. 10c-10f, 50 additional grains are assigned the properties of recrystallized tungsten each time, up to a point where the microstructure is fully recrystallized in Fig. 10f. In each microstructure, the crystal orientations of the recrystallized grains remain unchanged, consistent with the experimental observations made in Fig. 4a and Fig. 4b. This also allows for a more systematic simulation approach.

Figure 10: Microstructures with a monotonically increasing volume fraction of recrystallized grains. Blue: rolled material properties, red: recrystallized material properties.

The randomly selected grains in Fig. 10a-10f that are considered to be recrystallized have a volume percentage of 0%, 30.4%, 44.4%, 61.7%, 79.8% and 100% respectively. On these six microstructures, a similar analysis is performed as carried out in Sec. 6.1. Here, the BDTT is evaluated for different failure probabilities at 1% of strain, and the volume of the macroscopic specimen equals the one used in the experiments of Shen et al. [28], i.e. $V_{sp} = 5 \times 1.5 \times 0.75 \text{ mm}^3$. Upon recrystallization, a clear trend can be observed as shown in Fig. 11.

The brittle-to-ductile transition temperature is found to decrease linearly by about 200 K for a 100% volume fraction of recrystallized grains. Note that this linear dependence is almost independent of the failure probability used to define the BDTT. The brittle-to-ductile transition of the fully recrystallized microstructure in this analysis is different from what was reported in Sec. 6.1 due to the difference in specimen volume in the experiments of Younger and Wrights (1970) [26].

6.3. Transition zone

In this section, the failure probability of several configurations of the transition zone is investigated. Fig. 12a shows the microstructural configuration that is directly based on the EBSD scan in Fig. 1. Here, a similar procedure is adopted as presented in Sec. 3, but now also the recrystallized part of the

Figure 11: Decrease in brittle-to-ductile transition temperature at 1% strain with an increasing volume fraction of recrystallized grains.

microstructure is taken into account. Grains are considered to be recrystallized if the grain orientation spread is less than 3 degrees.

Figure 12: Several configurations of a partly recrystallized microstructure. The blue grains have the properties of rolled tungsten while the red grains have the properties of recrystallized tungsten. All crystal orientations are shown in TD.

In order to investigate what kind of transition zone is most favourable in terms of risk for brittle fracture, several configurations are considered. In Fig. 12b, the grains are assigned random coordinates as initial guess in the algorithm presented in Sec. 3, causing the rolled grains and recrystallized grains to be fully mixed. In Fig. 12c, the rolled grains and recrystallized grains are separated as much as possible, minimising the surface between these two types of grains.

The orientation distribution functions of the configurations are nearly identical, because they use the same set of crystal orientations and follow the same grain size distribution. The presented configurations in this section are subjected to 3D periodic boundary conditions. Furthermore, they are loaded in tension in various directions in the HD-TD plane. The angle under which the tensile loading is applied is characterized by ϕ , where $\phi = 0^\circ$ is parallel to HD and $\phi = 90^\circ$ is parallel to TD, see Fig. 13. The loading directions are applied in steps of 15 degrees.

In Fig. 13, the red line shows the failure probability of the fully mixed RVE shown in Fig. 12b. The anisotropic response is primarily due to the texture. In this configuration, the failure probability is the lowest when the RVE is loaded in HD, and gradually increases when the loading direction is rotated towards TD. The influence of the texture is investigated into more detail in Sec. 6.4.

Fig. 13 also shows that when the RVE consists of grains that are clearly spatially separated, the anisotropy of the probability of failure is significantly more pronounced. When the RVE is loaded under 45° , the failure probability is considerably lower compared to loading parallel to TD. In Fig. 14a, the EBSD based transition zone is loaded in horizontal direction (TD). The rolled and recrystallized parts of the RVE are now practically loaded in parallel. Since the rolled part has a significantly higher yield stress, this part is more stiff than the recrystallized part and hence relatively high stress levels result. In

Figure 13: Failure probability of the RVE for several transition zone configurations and loading directions at 1% strain.

Figure 14: Maximum stress on the $\{100\}$ family of cleavage planes, while loading in different directions. The nodal displacements are magnified by a factor 10.

Fig. 14b, the RVE is loaded in vertical direction. Now, the rolled and recrystallized parts of the RVE are loaded in series. However, due to the periodic boundary conditions, the lateral contractions in both the recrystallized part and the rolled part of the RVE are constrained to be the same. This causes a relatively large volumetric loading in the recrystallized part of the RVE, resulting in a relatively large failure probability on all three cleavage planes. If the RVE is loaded under 45° , the lateral constraint is not present, see Fig. 14c. Here, most of the deformation is absorbed by the recrystallized part of the RVE, resulting in a low and homogeneous stress field, with the exception of a few stress concentrations close to the interface.

6.4. Strongly anisotropic texture

Zhang et al. [32] showed that a highly anisotropic texture can be obtained from rolling high purity tungsten. The texture they presented is significantly more anisotropic compared to what was shown in Fig. 4 of the current work. The influence of such a strongly anisotropic texture on the probability of failure of an RVE is investigated in this subsection. To this end, the texture of the uniaxially rolled tungsten specimen from Zhang et al. [32] is mimicked by assigning small random perturbations to crystals that have the $\langle 100 \rangle$ axis aligned with TD. These crystal orientations are randomly assigned to the grains in the RVE presented in Sec. 3. The resulting pole figures are shown in Fig. 15.

The RVE is subjected to 3D periodic boundary conditions and is uniaxially loaded in different directions in the TD-HD plane, as shown in Fig. 16. The angle under which the tensile loading is applied is

Figure 15: Pole figures of a strongly anisotropic texture, mimicking the texture presented by Zhang et al. [32].

again defined by ϕ . The loading is applied in steps of 10 degrees. In each of these directions, the yield stress is shown by the red line, which is determined by considering the true stress at 0.2% plastic strain offset in the direction of loading.

Figure 16: Anisotropic response of the RVE, to which the texture shown in Fig. 15 is assigned. A high yield stress does not necessarily result in a high failure probability.

Clearly, the yield stress is rather anisotropic due to the strong texture. In the current work, slip is restricted to the $\{\bar{1}01\}\langle 111 \rangle$ family of slip systems. Therefore, a high yield stress is observed when the RVE is loaded at $\phi \approx 35^\circ$ because then a significant volume fraction of the grains is loaded in the $\langle 111 \rangle$ family of crystal directions which corresponds to the lowest Schmid factor.

In Fig. 16, the failure probability of the RVE is shown in blue. By comparing the red and blue curves, the competition between two mechanisms can be observed. While the yield stress is governed by the orientation of the slip directions and slip plane normals, the failure probability is governed by both the (yield) stress and the orientation of the cleavage planes. Although in TD the yield stress is relatively low, in this direction the failure probability is the largest because the crystals are mostly loaded normal to their cleavage plane. Accordingly, a high yield stress does not necessarily result in a high failure probability, because it also depends on the orientation of the cleavage planes with respect to the loading direction.

7. Discussion & Conclusions

The high temperature material properties of pure tungsten are compelling in terms of its application in plasma facing components for nuclear fusion reactors. Its low temperature behaviour is a source of concerns, emanating from the increasing risk for brittle failure with decreasing temperature. The brittle-to-ductile transition temperature is dependent on the tungsten microstructure, which evolves under

fusion conditions. In the current work, a framework is presented that allows to simulate this transition for various microstructural configurations.

The simulation results reveal a clear agreement with the brittle-to-ductile transition temperature observed in literature. Furthermore, it is shown that the brittle-to-ductile transition temperature of a rolled microstructure decreases with recrystallization, which is in line with several experimental results in literature [27, 33–35]. However, under fusion conditions, the tungsten plasma facing components are also subjected to neutron irradiation, which is well known to make tungsten more brittle. This competing effect is not taken into account in the current analysis. In the work of Németh et al. [6] and in Nikolić et al. [36] the opposite trend is observed, as their results show that the brittle-to-ductile transition temperature increases with recrystallization. This may be caused by the significant increase in grain size upon recrystallization. The brittle-to-ductile transition temperature is well known to be dependent on the grain size, which is not included in the framework presented in this work. However, the rolled and the recrystallized material currently investigated, have a similar grain size. Furthermore, the presence of impurities and the change in texture might trigger a different failure mechanism where cracks propagate on the grain boundaries.

The results also show that at constant temperature, the risk for brittle failure is higher for larger specimens because there is a higher probability of encountering a relatively large crack. The brittle-to-ductile transition temperature of these larger specimens is therefore also higher. The current simulation results show that the risk for brittle fracture is strongly related to the orientation of the cleavage planes with respect to the loading direction, which is frequently disregarded in literature.

The results also indicate that the brittle-to-ductile transition temperature decreases linearly with the recrystallized volume fraction. Here, it is assumed that there is a perfect mixture between the rolled and recrystallized grains. Finally, it is also found that the spatial separation of these phases only influences the risk for brittle failure if the specimen is loaded under an angle of approximately 45 degrees with respect to the normal of the plane of separation.

This work considers high-purity tungsten where the role of the grain boundary strength can be disregarded. Therefore, the cleavage fracture model describes only intra-granular failure, which is consistent with the experimental observations made by Shen et al. [28]. In the work of Younger and Wrights [26], the type of cleavage is not discussed. However, in the work of Sheng et al. [27], high purity recrystallized tungsten is considered as well, and they also observed intra-granular failure in the brittle regime.

Note that a worst case scenario was simulated here. In this regard, a microscopic crack subjected to an excessive stress automatically results in failure of the whole structure. A possible crack tip arrest due to micro structural barriers is disregarded. An interesting topic for future work would be to investigate the interactions between microcracks by progressively adding them to the RVE. Furthermore, the presented theory only applies to structures for which it holds that at constant load, the stress intensity factor increases with crack length. In the current work, the size-dependent specimen failure probability is calculated, taking into account the size of the experimental specimens. Here, it is assumed that the stress state is homogeneous on the macroscopic scale, which is not the case in a monoblock under fusion conditions. This can be accounted for in an integral sense, however, it is unlikely that local fracture will automatically result in functional failure of the monoblock.

The failure probability of a reference volume was linked to the underlying microstructure in the work of Mathieu et al. [10]. In order to identify at what instant failure occurs in the RVE, Mathieu et al. [10] considered a distribution of defects in the material. The largest defect in each grain is assumed to dictate its critical stress level. Mathieu et al. [10] assumed that failure would occur if the average stress in any of the grains exceeds its respective critical level. By considering a large number of realisations of defect distributions, the probability of failure of the reference volume could be estimated for a given macroscopic stress level. In order to perform this type of analysis, it is mandatory to gather detailed information of the microscopic defects in terms of density, size distribution, shape and surface energy. In the current work, these quantities are unknown and are all collected under a single parameter σ_{ref} , which is a simplified measure for the material's resistance to cleavage.

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