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Microstructural evolution and regeneration in neutron-irradiated tungsten monoblocks

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ABSTRACT

The lifetime of the divertor in tokamak nuclear fusion reactors is uncertain, due to the severe heat, ion and neutron loads that are imposed on the plasma-facing monoblocks, which are made of tungsten. In this work, the microstructural evolution throughout the monoblock is modelled, using a multi-scale model that spans from displacement damage evolution to macroscopic material properties and temperature profiles. The evolution of the hardness and the thermal conductivity as a function of monoblock depth are studied, under a combination of heat and neutron loading, based on the concentrations of the radiation-induced defects. An increase of the temperature gradient over the monoblock is predicted, which entails serious consequences for the magnitude of the thermal stresses and the accompanying surface temperature. For the selected parameter set, the high surface temperature leads to recrystallization of a small layer of material near the surface, locally reducing the amount of irradiation hardening. Interim heat treatments of 1 h are simulated, which evoke recrystallization in the monoblock and which either reset the accumulated irradiation hardening, or keep it low, throughout the monoblock, thereby increasing the ductility again, and proving that such treatments could be a valuable tool on the way to prolongation of the lifetime of these monoblocks.

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1. Introduction

Currently, mankind is facing a transition from electricity generation from non-renewable fuels to more sustainable sources. Electricity generation powered by nuclear fusion would largely help solve the energy problem in society. A critical component in a Tokamak fusion reactor is the divertor, which receives the highest heat load ($\sim 10 \text{ MW/m}^2$ for ITER in steady state (Carpentier-Chouchana et al., 2014) and perhaps similar for DEMO (You et al., 2018)) of all plasma-facing materials. On top of that, there is also a significant neutron load ($\sim 4 \times 10^{-8}$ displaced atoms/s (Mannheim, van Dommelen, & Geers, 2018), based on Gilbert, Marian, and Sublet (2015) and Setyawan et al. (2015)), as well as continuous ion irradiation. For economical reasons, the divertor should stay functional, and mechanically intact, for at least 2 full power years until replacement in the case of DEMO (You et al., 2016).

The plasma-facing part of the ITER divertor consists of 2×10^5 monoblocks, which are made of tungsten. The tungsten surrounds a cooling tube, consisting of a Cu-interlayer and a CuCrZr-tube, which contains the cooling water. The tungsten acts as an armour for the cooling tube, protecting it from the severe plasma irradiation. The required thickness of the

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tungsten monoblocks is based on the expected erosion rate that occurs during ion sputtering. The high heat flux through the monoblock leads to a strong temperature gradient over the monoblock. This induces thermal stresses that cause severe mechanical loading of the monoblocks. Moreover, during operation, the macroscopic thermo-mechanical material properties of the tungsten will change due to irradiation-induced damage within the microstructure.

For the prediction of the evolution of the material properties throughout the tungsten block, the combined effect of the heat and neutron load is important, whereas the ion irradiation mainly affects the surface. The neutron irradiation generates atomic displacement cascades (leading to the formation of lattice defects) and induces transmutations (Was, 2007). The displacement damage affects the mechanical material properties, through irradiation hardening (Zhang, Hasenhuettl, Yabuuchi, & Kimura, 2016), embrittlement (which accompanies the hardening) and by elevating of the ductile to brittle transition temperature (DBTT, Bolt et al., 2002). Moreover, the neutron irradiation will lead to swelling (Matolich, Nahm, & Moteff, 1974) and creep. This evolution of the material's structure and properties under neutron irradiation depends strongly on the irradiation temperature.

The effect of neutron displacement damage (such as vacancies, self-interstitial atoms and dislocations) on the thermal material properties of tungsten is often assumed to be negligible (Barabash, 2013; Tolias & EUROfusion MST1 Team, 2017). However, there are convincing indications that the displacement defects lead to a significant decrease in the thermal conductivity: (1) severe cold working of tungsten (wire drawing) was shown to lead to an increase of the electrical resistivity (Broom, 1952) of 50%, and (2) several recent measurements on the thermal diffusivity and thermal conductivity of irradiated tungsten (Cui et al., 2018; Habainy, Dai, Lee, & Iyengar, 2018). Thermal diffusivity measurements by Habainy et al. (2018) indicate that the displacement damage significantly affects the thermal conductivity. Habainy et al. measured the thermal diffusivity change of tungsten as a consequence of proton irradiation in combination with fast neutron irradiation to 3.8 dpa (leading to 2 wt.% Re). To distinguish the contributions of the transmutations and the displacements, they performed measurements before and after annealing the sample for 1 h to 1000 °C, and found 28–51% recovery of the thermal conductivity by annealing. Furthermore, Cui et al. (2018) measured a 20% reduction of the thermal conductivity at the tungsten surface following 0.2 dpa of ion-irradiation of tungsten at 1000 K, which can be attributed purely to displacement defects.

A continuous decrease of the thermal conductivity during neutron load leads to an increasing temperature at the surface of the monoblock. This also means that an increasing part of the monoblock material will approach or exceed the recrystallization temperature, and that due to the increased temperature gradient inside the monoblock, the thermal stresses increased.

The combination of high temperatures and displacement damage makes recrystallization and grain growth likely to occur. Usually, for metals, recrystallization leads to an increase in ductility and a decrease in strength (Humphreys & Hatherly, 2004). Sometimes, recrystallization of tungsten is presumed to cause embrittlement (Babak & Uskov, 1984), which should be avoided. In any case, it may prove difficult to avoid the occurrence of recrystallization in the monoblocks, as the increasing material damage leads to an increase of the DBTT and also to a decrease of the recrystallization temperature, so the operation temperature window in which it can be avoided continuously shrinks.

However, several studies contradict the embrittlement hypothesis and indicate an increase of the ductility of tungsten after recrystallization. In Barabash (2013) and Davis, Barabash, Makhankov, Plöchl, and Slattery (1998), a remarkable increase of the total elongation is reported after recrystallization, over the entire temperature ranges measured (500–1800 °C and 500–2500 °C, respectively). Also in Wirtz, Uytdenhouwen et al. (2017) and Wirtz, Kreter et al. (2017), a significantly increased total elongation was reported. In a recent review paper by Marian et al. (2017), it is stated that the brittle behaviour of sintered tungsten under irradiation is most likely not an intrinsic property of tungsten, but rather an artefact that comes from grain boundary weakening caused by the processing method.

If this embrittlement can be avoided, recrystallization can actually be beneficial in a divertor monoblock, as it erases some of the detrimental effects of neutron irradiation.

To study the combined processes of neutron irradiation and recrystallization and grain growth, model simulations are necessary, because currently no experimental facility exists where the irradiation effects of 14 MeV neutrons on the material's structure can be mimicked (Knaster et al., 2014): fission neutrons have a different energy spectrum and therefore create too many transmutations, while (self-)ions affect only a volume of ~ 300 nm thick, which is too small to test the thermo-mechanical bulk material properties. Moreover, surface effects play a dominant role in this region. Simulations were performed in Mannheim et al. (2018) to study the combined effect of heat and neutrons, using a multi-scale model that consists of a cluster dynamics model for the neutron displacement damage in the grains, coupled to a mean-field recrystallization model which describes the evolution of recrystallization and grain growth. Cyclic neutron-induced recrystallization was predicted to occur for irradiation temperatures of 1000–1300 °C (Mannheim, van Dommelen, & Geers, 2019a). Clear indications were found that the cyclic recrystallization limits the irradiation hardening considerably. The results in Mannheim et al. (2018) also showed the strong temperature dependence of the competition between the occurring damage and recovery mechanisms. The modelling framework was used to explore the effects of intermittent heat treatments in the temperature range of 800–1000 °C, as a means to systematically reduce the severe irradiation hardening (Mannheim, Dommelen, & Geers, 2019b).

In this paper, the microstructural evolution over the entire thickness of the monoblock as a consequence of neutron displacement damage and heat is studied using an extended multi-scale model which includes thermal coupling, yielding a spatial distribution for the microstructural properties. The temporal and spatial variations of two characteristic thermo-mechanical material properties, *i.e.* hardness (which is used as a predictor for the ductility) and thermal conductivity, are

studied. Due to the thermal coupling, the change of the thermal conductivity directly affects the (strongly temperature dependent) microstructural evolution. An investigation of the effects of possible lifetime-improving heat treatments on the entire monoblock is performed, taking benefit of the rejuvenating effect of recrystallization.

2. Modelling framework

2.1. Problem statement

The microstructural evolution along the center line of a divertor monoblock is studied, by simulating the heat and neutron effects in a volume of bulk tungsten of 8 mm in thickness. The material receives a heat flux of $q_{in} = 10 \text{ MW/m}^2$ at the top surface, and is cooled at the bottom. From (Panayotis, 2015), it is clear that the steady-state temperature distribution over the monoblock is reached in less than 10 s after heating is started. Since in this work, the microstructural evolution will take place on much longer time scales, it is assumed that the steady-state temperature distribution is obtained instantaneously and that the heat influx q_{in} equals the heat outflux q_{out} at all times. The temperature at the bottom of the tungsten is taken to be 380 °C, based on the simulation results in Panayotis (2015) with a similar heat load. On top of the heat load, the entire monoblock receives neutron irradiation, which leads to $3\text{--}4 \times 10^{-8}$ displaced atoms/s in the tungsten, depending on the temperature, see Section 2.3.

2.2. Multi-scale model

The microstructural evolution in the monoblock as a consequence of the heat and neutron loads is described with a multi-scale model, which is schematically depicted in Fig. 1. The heat load at the surface in combination with the cooling creates a temperature gradient over the tungsten block, leading to a different temperature at different depths along the center line of the block. Neutron irradiation leads to damage accumulation in the individual grains. Depending on the temperature, rejuvenation takes place locally, in the form of: Clustering of defects (Li et al., 2012), defect annihilation (Li et al., 2012) at sinks or annihilation of vacancies with self-interstitial atoms, defect sweeping during grain growth (Bernard, Bag, Huang, & Logé, 2011) and nucleation of new grains (Bernard et al., 2011).

At the macroscopic level, the spatial temperature distribution $T(x)$ is modelled using the local thermal conductivities $k_{th}(x)$. The local temperature determines the rate of the various microstructural recovery processes.

At the mesoscopic level, the local changes in grain size $r_{g,k}$ and defect concentrations C_k and dislocation densities ρ_k for a set of k representative grains in each material point l at the macroscopic level is modelled, using a mean-field recrystallization model (Bernard et al., 2011; Mannheim et al., 2019b). These changes are the consequence of grain growth and nucleation.

Fig. 1. Schematic representation of the multi-scale model for the thermally coupled microstructural evolution under combined heat and neutron loads. Here, $q_{in} = q_{out}$ denotes the heat flux (W/m^2) that is conducted through the material. Each material point has a different temperature, inducing a thermal gradient at sufficiently high temperatures. Interactions between the grains can lead to nucleation of new grains and grain growth. Meanwhile, neutron damage is induced in the individual grains with evolving damage concentrations.

At the microscopic level, the production and evolution of the defect concentrations in all of the representative grains of each material point, is modelled using cluster dynamics. These defects occur as a consequence of atomic displacements that are induced by bombardments of the atoms with fast neutrons. These defects interact with each other, leading to clustering or annihilation.

2.2.1. Coupling

The following types of displacement defect concentrations are considered at the microscopic level: vacancies C_V , vacancy clusters of size n , C_{V_n} , self-interstitial atoms C_I , self-interstitial atom clusters of size n , C_{I_n} and the dislocation network density ρ . These defects represent a particular contribution to the stored energy in the crystal lattice, which drives nucleation and grain growth at the mesoscopic level (Mannheim et al., 2018), which in turn affects the defect concentrations. Also, the defect concentrations determine the local thermal conductivity k_{th} , which will affect the macroscopic temperature distribution.

Below, the three parts of this multi-scale model are presented. For each part, the physical mechanisms of the model are set out. The cluster dynamics model and the recrystallization model have been extensively described in Mannheim et al. (2018, 2019a, 2019b) and are therefore only discussed briefly. Computational details can be found in Appendix A and Appendix B.

2.3. Neutron-induced lattice damage

The production and evolution of neutron-induced defects in single grains is modelled using cluster dynamics (Li et al., 2012; Mannheim et al., 2019a). An overview of the processes that are accounted for in the model, is shown in Fig. 2. The production originating from displacement cascades caused by neutrons (Yi et al., 2015) and evolution of the defect concentrations in the grains over time are predicted, using a set of coupled differential equations, see Appendix A for details. The evolution of the dislocation density and of the concentrations of vacancies (V) and self-interstitial atoms (SIAs) and

Fig. 2. Overview of the cluster dynamics model, showing which defect concentrations inside a grain are produced by neutron irradiation and how they are evolving, along with the physical processes driving the evolution.

their clusters is modelled, where SIA-clusters are assumed to be planar defects and V-clusters are assumed to be spherical (Li et al., 2012). The single vacancies (V_1) and single SIAs (I_1) are the only defects that are considered to be mobile.

The following processes are incorporated in the model, see Fig. 2:

- The production of the defects (1), which is temperature dependent (Setyawan et al., 2015).
- Following their production, the defect clusters can change in size, during absorption and emission of mobile defects (2).
- The mobile defects can also be absorbed by grain boundaries (3) (which introduces a grain size dependence),
- annihilate with their opposite defect (together V_1 and I_1 are a Frenkel pair)(4),
- or be absorbed by dislocations (5).

The rates of these processes are temperature dependent, because the diffusivity of the mobile defects is temperature dependent as well as the attempt frequency for a mobile defect to be emitted from its cluster. Meanwhile, the dislocation density evolves by dipole annihilation (by climb) (a) and by pinned dislocation segments that form Bardeen-Herring sources (b), which operate by climb. The climb velocity is temperature dependent and also depends on the concentrations of the mobile defects.

2.4. Mean-field recrystallization model

The high temperatures and high concentrations of irradiation defects drive the evolution of the microstructure through recrystallization and grain growth. These processes are modelled using a mean-field recrystallization model (Bernard et al., 2011). The microstructure in a material point is described with a set of k representative grains, which interact with a number of homogeneous equivalent media (HEMs) (Mannheim et al., 2019b). The representative grains are spherical in shape with properties: $r_{g,k}$ (grain radius), C_k and ρ_k (defect concentrations and dislocation density) and N_k (the number of grains they represent in the microstructure). Note that the non-topological nature of the model makes it computationally feasible to use it within the multi-scale model.

The microstructure contains stored energy due to lattice defects in the bulk of the grains (E^B) and at the grain boundaries (E^S). The difference between the stored energy of a grain and that of the HEMs determines the velocity of the shared grain boundary segments.

The stored energy in the microstructure also determines the nucleation activation energy and the radius of a stable nucleus. It is assumed that new grain nuclei form at grain boundaries, as observed for static recrystallization by Lopez (2015). Nucleation in the bulk of the grains has been studied in Mannheim et al. (2019a). The model contains parameters for the grain boundary mobility, the nucleation rate and the nucleation activation energy, which have been characterized using static recrystallization experiments on tungsten (Mannheim et al., 2019b).

During nucleation, a defect-free lattice volume is formed consuming a defected lattice (Humphreys & Hatherly, 2004). Furthermore, during grain growth, the grain boundaries move and sweep the defects on their path, leaving behind near-perfect crystals. A schematic illustration of these processes is given in Fig. 1. Thereby, nucleation and grain growth lead to a reduction in the stored energy in the lattice. Details can be found in Appendix B and a more elaborate discussion of the model can be found in Mannheim et al. (2019b).

2.5. Thermal problem

In steady state, the spatial temperature distribution along the depth of a tungsten monoblock is described by a one-dimensional model:

$$\frac{\partial}{\partial x} \left(k_{th}(x) \frac{\partial T}{\partial x} \right) = 0, \quad (1)$$

with boundary conditions:

$$k_{th}(x_0) \frac{\partial T(x_0, t)}{\partial x} = -q_{in}, \quad (2)$$

$$T(x_L, t) = T_L. \quad (3)$$

Here, x is the distance to the surface of the monoblock, k_{th} is the thermal conductivity, $q_{in}=10 \text{ MW/m}^2$ is the heat flux that enters the divertor's surface at $x=x_0$, x_L is the position of the interface of tungsten with the cooling tube at the center line of the monoblock and T_L is the temperature at this location. Eq. (1) is discretized in space and is solved using a finite difference scheme. This gives:

$$T(x_{j+1}) = T(x_j) + \frac{q_{in}}{k_{th}(x_j)} (x_{j+1} - x_j). \quad (4)$$

Here, x_j is the position of node j , $T(x_j)$ is the temperature at position x_j and $k_{th}(x_j)$ is the thermal conductivity at x_j .

2.5.1. Thermal conductivity

The thermal conductivity for metals is closely related to their electrical resistivity. For pure metals, the electrical resistivity is given by [Hust and Giarratano \(1975\)](#):

$$\rho^{el}(T) = \rho_0^{el} + \rho_i^{el}(T). \quad (5)$$

Here, ρ^{el} is the electrical resistivity in Ωm , ρ_0^{el} is the residual resistivity and ρ_i^{el} is the intrinsic resistivity. The first term is temperature-independent, and is caused by electron scattering with chemical impurities and physical imperfections in the material (defects), while the second term is due to electron-phonon scattering, which is a temperature-dependent process.

Expressions for the thermal conductivity k_{th} (in W/mK) depend on the residual resistivity were developed by NIST (which in their case is a function of impurity content) ([Hust & Landford, 1984](#)):

$$k_{th} = (W_0 + W_i + W_{i0})^{-1}, \quad (6)$$

with

$$W_0 = \frac{\rho_0^{el}}{TL_0}, \quad (7)$$

where T is the temperature in Kelvin and $L_0 = (\pi^2/3)(k_B/e)^2 = 2.443 \times 10^{-8} \text{ W}\Omega/\text{K}^2$ the Sommerfeld value of the Lorenz ratio ([Klemens, 1989](#)) with e the electrical charge, and

$$W_i = \frac{P_1 (T/T_{ref})^{P_2}}{1 + P_1 P_3 (T/T_{ref})^{P_2+P_4} \exp(-(P_5 T_{ref}/T)^{P_6})} + W_c, \quad (8)$$

$$W_{i0} = \frac{P_7 W_i W_0}{(W_i + W_0)}, \quad (9)$$

where the values of the parameters $P_1, \dots, P_7$ and T_{ref} are given in [Table 5](#) in [Appendix C](#), along with the empirical function W_c ([Hust & Landford, 1984](#)). [Eq. \(6\)](#) was also recommended to be used for the calculations for ITER ([Tolias & EUROfusion MST1 Team, 2017](#)) (in there, the residual resistivity ρ_0^{el} is taken such that the residual resistivity ratio ($= \rho_{300K}^{el}/\rho_{0K}^{el}$) = 300, which corresponds to a material with a low concentration of defects).

The intrinsic electrical resistivity ρ_0^{el} of the material is determined by all the defects (impurities, grain boundaries, displacement defects and dislocations). The specific dislocation resistivity (resistivity due to a single unit of dislocation length per unit volume) has been measured at low temperatures to be $\Re_d = 6 \times 10^{-25} \text{ }\Omega\text{m}^3$ ([Watts, 1988](#)). The electrical resistivity due to dislocations is then given by:

$$\rho_0^{el,d} = \Re_d \rho, \quad (10)$$

with ρ the dislocation density. According to [Karolik and Luhvich \(1994\)](#), the grain boundary resistivity of tungsten is $2.0 \times 10^{-15} \text{ }\Omega\text{m}^2$, which may induce a small decrease in thermal conductivity¹, which is however neglected here. Furthermore, the vacancy and interstitial defects are expected to contribute to the resistivity, but no specific information allowing to quantify this effect is available at present. The contribution is therefore taken to be equivalent to the dislocations, based on their stored energy, leading to:

$$\rho_0^{el} = \Re_d \frac{E^B}{\frac{1}{2} \mu b^2}, \quad (11)$$

where E^B is the bulk stored energy, μ is the shear modulus and b is the Burgers vector.

2.6. Hardness

Based on the Dispersed Barrier Hardening-model ([Hu et al., 2016](#)), a hardness indicator was formulated previously ([Mannheim et al., 2019a](#)), and used to study the evolution of the hardness during the microstructural evolution. The lattice defects are considered to be obstacles that obstruct glide of dislocations. Depending on the defect size and type, the defect forms a stronger or weaker barrier, which is expressed using the barrier strength factor α . The hardness indicator is given by

$$\mathcal{H}_H = \frac{\sqrt{\rho} + \frac{M}{\alpha_T} \sqrt{\sum_j 2\alpha_j^2 C_j r_j}}{\sqrt{\rho_0}}, \quad (12)$$

where the barrier strengths α_n correspond to defect clusters of size n and the defect radius r_n can be found in [Table 1](#). In [Eq. \(12\)](#), α_T is the dislocation barrier strength and M is the Taylor factor, see [Appendix C, Table 5](#). All parameters are temperature-independent.

¹ A grain radius of $3 \mu\text{m}$ would give $\rho_0^{el} = 2 \times 10^{-9} \text{ }\Omega\text{m}$. From [Eq. 6](#), this gives a thermal conductivity which is 3.5% lower than in the defect-free case, at $T = 380^\circ \text{C}$ (which is the minimum value that occurs in the thermal problem of this paper).

Table 1

Barrier strengths in the DBH-model for the corresponding cluster sizes. For clusters of smaller sizes, $\alpha = 0$ is taken (Hu et al., 2016).

	Barrier strength factor α	Diameter (nm)	Cluster size N
Interstitial loop	0.15	1.0–2.7	14–100
Void	0.25	1.0–1.4	33–100

Fig. 3. (a) Nodal positions of the 13 material points in the monoblock. Their precise spatial locations can be found in the Section 3; (b) Sketch of the solution procedure for the multi-scale model. At each time increment, the temperature distribution over the monoblock is determined based on the defect densities. Next, for each NIRX-material point l , the cluster dynamics model (CD) and the recrystallization model (RX) are used sequentially to update the microstructural parameters for the representative grains k that constitute the microstructure. The (volume averaged) defect concentrations of the NIRX-points are interpolated for the other points.

2.7. Solution procedure

The geometry consists in total of $P = 801$ equally separated macroscopic material points, which are located at $x_0 = 0$ mm up to $x_L = 8$ mm. In 13 of these points, which are adequately distributed over the monoblock center line (see Fig. 3(a)), the model for neutron-induced recrystallization (NIRX) is applied. For all other points, linear interpolation of the defect concentrations is used to determine the local thermal conductivity, which governs the temperature profile. The solution procedure for the multi-scale model is illustrated in Fig. 3(b).

The following steps are repeated until the final simulation time has been reached:

1. The size of the time increment $\Delta t = t_{i+1} - t_i$ is determined. The time step size is constrained such that only moderate amounts of grain growth, nucleation, heating and defect accumulation occur within a single increment.
2. Based on the current defect concentrations in each of the 13 NIRX-nodes, the thermal conductivity and temperature distribution are determined.
 - First, the volumetric average of the defect concentrations in each material point is determined.
 - To estimate the residual resistivity due to all defects, the bulk stored energy is calculated for the NIRX-nodes, using Eq. (11).
 - Interpolation is used to estimate ρ_0^{el} for all other nodes.
 - Eq. (6) is used to calculate the thermal conductivity $k_{th}(x_l)$ in each material point x_l .
 - Eq. (4) is solved to calculate the temperature profile $T(x_l)$.
 - In case of an intermittent heat treatment, the temperature profile is prescribed, using a ramp time of 600 s, and no neutron irradiation is applied. During the ramp time, the temperature is increased (or decreased) linearly, based on the thermal conductivity for the momentary defect concentrations.
3. The neutron-induced recrystallization-calculation is performed separately for each NIRX-node, which results in updated microstructural properties ($C_{n,k}$, $C_{Vn,k}$, ρ_k , $r_{g,k}$, N_k) for all k representative grains in the microstructure at material node l , and for cluster sizes $n = 1 \dots N_{max}$. The complete NIRX solution procedure is described in more detail in Mannheim et al. (2019b).

3. Results

The simulation results for the microstructural evolution along the depth of the monoblock under neutron irradiation and heat are presented. Section 3.1 reports the results under constant heat loading; Section 3.2 describes the effects of the intermittent heat treatments. For the initial microstructure, a normal grain size distribution is assumed, with an average radius of $r_g = 3 \mu\text{m}$ and a standard deviation of $0.5 \mu\text{m}$. Thermal equilibrium defect concentrations (based on the defect formation energies) for the vacancy and interstitial defects and a dislocation density of $1 \times 10^{13} \text{ m}^{-2}$ are assumed for the initial state.

Fig. 4. Temporal evolution of (a) the thermal conductivity k_{th} , (b) the temperature T , (c) the stored energy E^B , (d) the hardness indicator I_H , (e) the average grain size r_{avg} along the thickness of the monoblock; (f) evolution of the recrystallized fraction over time at all NIRX-nodes. f^{RX} denotes that no original grains remain left in the microstructure.

3.1. Steady-state spatial evolution

In Fig. 4, the resulting evolution of the microstructure at various depths of the monoblock is shown. Over time, the temperature gradient over the block increases (Fig. 4(b)) due to the decreasing thermal conductivity (Fig. 4(a)). The thermal conductivity decreases most at larger depths, where defect concentrations are highest since less recovery took place (lower mobility of the defects and grain boundaries). The temperature at the surface of the monoblock has raised by more than 60 °C, from 1045 °C to 1106 °C.

Fig. 5. Evolution of the stored energy E^B at the NIRX material points along the thickness of the monoblock under (a) constant neutron irradiation and heating and (b) neutron irradiation and intermittent heat treatments at 1200 °C every 100 hrs, as a function of simulation time t . The evolution of the hardness indicator T_H over time is shown for all NIRX-points, during constant heat loading and neutron irradiation, in (c), and with intermittent heat treatments, in (d).

The evolution of the hardness (Fig. 4(d)) largely follows that of the bulk stored energy E^B (Fig. 4(c)), except at larger depths (> 5.5 mm) where lower irradiation temperatures are endured, point defects undergo less clustering. The smaller clusters form less effective obstacles and do not affect the hardness much, while they do contribute to the bulk stored energy. The maximum increase of the hardness indicator after 600 h of irradiation is found at a depth around 5.5 mm from the monoblock's surface.

Fig. 4(e) and f reveal that recrystallization and grain growth take place near the surface of the monoblock. After 600 h, the first 1.5 mm of the block has recrystallized. At this time instance, recrystallization starts to take place at the node located at 2 mm. At this node, the temperature has increased from initially 868–927 °C over the course of the 600 h of irradiation.

Summarizing, recrystallization takes place in the region of 0–2 mm (entailing a reduction of defects in that region), whereas this would be most desired in the region of 4–8 mm, where the increase of the hardness indicator is the highest. Therefore, heat treatments for regeneration of the microstructure may be an interesting option to reduce the embrittlement within the monoblock.

3.2. Heat treatment effects

The effect of interim heat treatments on the microstructural evolution of the tungsten monoblock is investigated. In Fig. 5, a comparison is shown for the evolution of the bulk stored energy E^B and the hardness indicator T_H under the following operation conditions: (1) continuous loading with neutrons and 10 MW/m² of heat, (2) same loading condition, but with 1 h of intermittent annealing at 1200 °C and no neutron irradiation, repeated every 100 h, which will be referred to as the heat treatment case. The 1 h of treatment is preceded and followed by 10 min. of ramp time, towards, or away from 1200 °C.

Fig. 5(a) and (b) show the evolution of the bulk stored energy E^B and temperature at the NIRX-points, for the continuous loading case and for the heat treatment case. The occurrence of recrystallization at depths of 0–1.5 mm is apparent from the evolution of E^B as a function of irradiation time in Fig. 5(a). The heat treatments (Fig. 5(b)) affect the microstructural evolution over the entire thickness of the monoblock: at the bulk of the block (2–8 mm), the heat treatments lead to a reduction of lattice defects and the bulk stored energy does not rise as high as for the continuous loading case. Near the surface, in the region of 0–1 mm, heat treatments are not necessary for recrystallization to take place. After 800 h, the stored energy levels that are reached are slightly higher for the heat treatment case, because these treatments lead to a

Fig. 6. Evolution of the spatial distributions of (a) the hardness indicator $\mathcal{I}_H$ and (b) the average grain size r_{avg} during the heat treatment. Temporal evolution of (c) the evolution of $\mathcal{I}_H$ and (d) the recrystallized fraction f^{RX} in all the NIRX-nodes during the heat treatment.

lower surface temperature, so that faster damage accumulation occurs when the neutron source is on) and less recovery takes place. At a depth of 1.5 mm, the obtained levels for the stored energy after 800 h are similar, with or without heat treatment. In the continuous loading case, more recovery takes place during irradiation (because of the higher irradiation temperature, which is due to the decreased thermal conductivity in the region 2–8 mm), while for the heat treatment case, short, sudden drops in the stored energy occur, after which damage accumulation resumes.

The application of the periodical heat treatment leads to significantly lower maxima for the hardness indicator in the monoblock, as shown in Fig. 5(c) and (d). Instead of reaching over 150 at 5.5 mm after 800 h of irradiation, $\mathcal{I}_H$ stays below 125 for all material points.

Now, the microstructural developments during the first heat treatment (starting after 100 h of irradiation) are investigated. Fig. 6(a) and (b) show the decrease in $\mathcal{I}_H$ and increase in grain size that occur during the annealing time, as a function of depth. During the treatment, $\mathcal{I}_H$ reduces to (nearly) zero at depths of 4–8 mm. At more shallow depths, recrystallization already partially took place before the start of the heat treatment (see Fig. 5(d)), whereby the accumulated damage since then is not sufficient for completing recrystallization, despite the elevated temperature. Nevertheless, during the heat treatment, the partial recrystallization is accelerated at 0–4 mm, and $\mathcal{I}_H$ decreases significantly in most of the nodes. After each heat treatment, $\mathcal{I}_H$ has dropped below 30 at all nodes. From Fig. 6(a) and (d), it can be observed that recrystallization occurs more rapidly at larger depths, entailing a larger decrease of $\mathcal{I}_H$. Indeed, at large depths the driving force for recrystallization is the highest. The average grain size after recrystallization is also higher at higher depths (Fig. 6(b)), where recrystallization occurs so fast that not many nuclei form. Fig. 6(c) shows sudden significant peaks of hardness increase for depths of 5.5–8 mm, while for 2–4 mm, there are no peaks at all. The peaks can be ascribed to the clustering of small defects that formed at low irradiation temperatures. The defect clustering occurs before recrystallization sets in.

4. Conclusions

The lifetime of the divertor is a main concern for realizing nuclear fusion reactors generating electrical power on a continuous basis. The divertor monoblocks are severely loaded with heat, neutrons and ions, and over time, the thermo-mechanical properties of the monoblocks are expected to degrade.

Here, the evolving material properties throughout the monoblock were studied, down from the microstructural evolution that occurs as a consequence of heat and neutron displacement damage (both affecting the bulk of the material, in

contrast to ion irradiation which is mostly confined to the surface). A multi-scale model was developed for this purpose, that describes (1) the neutron-induced damage evolution at the lattice level, (2) the microstructural evolution as a consequence of recrystallization and grain growth at the polycrystalline material point level and (3) the evolving thermal conductivity (dictated by the local neutron displacement damage) which governs the temperature profile over the monoblock.

The model was used to study the effect of neutron-induced displacement defects on the microstructural evolution and the thermal conductivity, and through the heat equation also the temperature distribution over the monoblock. Under continuous heat and neutron loading, the thermal conductivity was predicted to degrade significantly over time, leading to a steeper temperature gradient over the monoblock and a higher surface temperature. The thermal conductivity decrease was most severe deeper in the monoblock, close to the cooling tube. The irradiation-induced hardness appears to be the highest in this region as well. Meanwhile, near the surface, recrystallization and grain growth occurred, thereby accumulating less irradiation damage. Over time, the thickness of the recrystallized surface layer was observed to grow as a consequence of the increasing temperatures and ongoing damage accumulation.

Furthermore, it was investigated whether an intermittent heat treatment, triggering recrystallization throughout the entire monoblock, allows to reduce the irradiation hardening (especially deeper in the monoblock) in order to improve the material's ductility.

Every 100 h of irradiation, a heat treatment was applied during 1 h, using an annealing temperature of 1200 °C. At almost all instances, the hardness indicator over the entire spatial range decreased, to below 30, and full recrystallization was attained at depths of 5.5–8 mm in the monoblock after the first heat treatment, limiting the maximum value for the hardness indicator considerably (from over 150 after 800 h of continuous heat and neutron irradiation to less than 125). Deeper in the monoblock, rapid increases in the hardness indicator were observed at the start of the heat treatment, prior to recrystallization, as a consequence of massive clustering of the small irradiation defects (which had previously been nearly immobile due to the relatively low irradiation temperatures).

Note that, given the lack of sufficient experimental data, the multi-scale model only provides qualitative predictions. Nevertheless, this framework can be used to investigate possible scenarios in terms of design and engineering solutions. The physical mechanisms that are predicted are expected to occur also for different parameters in the model, albeit perhaps at different time scales or load levels. The model can serve as a primary tool for studying the effects of operating conditions, designs and initial microstructure on the evolving properties and functionality of the monoblock. Specifically, it was investigated here how heat treatments could affect the spatially varying evolution of the microstructure, the hardness and the thermal conductivity, enabling possible divertor lifetime improvements.

Even though an intermittent heat treatment has been shown to be useful, applying it still poses significant challenges. The current divertor design is based on the presence of a temperature gradient, with a lower temperature at the cooling tube. The material that was selected for the cooling tube (CuCrZr) will not be able to sustain the elevated temperatures during the heat treatments (its temperature window is in the range 180–280 °C (Fabritsiev, Zinkle, & Singh, 1996)). Also, texture and grain shape now play a role in the choice of the initial structure of the monoblocks, but the initial structure will be lost after recrystallization.

In the current model, only the combined effect of neutron irradiation and heat loads for relatively short time scales is considered. For longer time scales, additional effects of transmutations (composition changes and He production) due to neutrons are important. Except by transmutation, He is also implanted at the surface due to the plasma load. While it is known that He initially gets trapped in a small surface layer on short time scales, in the long term, helium diffuses into the bulk of the material. There, the helium will cluster with vacancies and voids and will also settle at dislocations and grain boundaries, thereby reducing the mobility of the grain boundaries. This will lead to a retardation of the recrystallization process (Guo, Cheng, De Temmerman, Yuan, & Lu, 2018).

The model predictions can be made more quantitative by performing validation experiments for the accumulation of the stored lattice energy across a wide temperature range and by studying the defect saturation levels. Also, experimental investigation of the recrystallization mechanisms and time scales under these conditions would be useful. Such experiments may be feasible in the future irradiation facility IFMIF. In the future, the model can be extended to include not only thermal coupling, but also the effects of the mechanical stress state on the evolution of the defects and the recrystallization process.

Declaration of interests

None.

Data availability

The data generated or analysed in this study are available upon simple request.

Appendix A. Cluster dynamics model

The following coupled set of differential equations describes the production and evolution of all the defect concentrations inside a grain (Mannheim et al., 2019a):

$$\begin{aligned} \frac{dC_I}{dt} = & G_I + k_{I_2+V}^+ C_{I_2} C_V + 2\alpha_2^- C_{I_2} + \sum_{n=3}^{N_I} \alpha_n^- C_{I_n} - 2\alpha_1^+ C_I^2 - \sum_{n=2}^{N_I} \alpha_n^+ C_I C_{I_n} - k_{I+V}^+ (C_I C_V - C_I^{eq} C_V^{eq}) \\ & - \sum_{n=2}^{N_V} k_{V_{n+I}}^+ C_I C_{V_n} - (k_{D+I}^+ + k_{S+I}^+) C_I \end{aligned} \quad (13)$$

$$\frac{dC_{I_2}}{dt} = G_{I_2} + \alpha_1^+ C_I^2 + k_{I_3+V}^+ C_{I_3} C_V + \alpha_3^- C_{I_3} + k_{I-V}^- C_I - \alpha_2^- C_{I_2} - \alpha_2^+ C_{I_2} C_I - k_{I_2+V}^- C_{I_2} - k_{I_2+V}^+ C_V C_{I_2} \quad (14)$$

$$\begin{aligned} \frac{dC_{I_n}}{dt} = & G_{I_n} + \alpha_{n+1}^- C_{I_{n+1}} + \alpha_{n-1}^+ C_I C_{I_{n-1}} + k_{I_{n-1}-V}^- C_{I_{n-1}} - \alpha_n^+ C_I C_{I_n} + k_{I_{n+1}+V}^+ C_V C_{I_{n+1}} - \alpha_n^- C_{I_n} - k_{I_n+V}^+ C_V C_{I_n} - k_{I_n-V}^- C_{I_n}, \\ & \text{for } \$3 \leq n \leq N_I - 2, \$ \end{aligned} \quad (15)$$

$$\begin{aligned} \frac{dC_{I_{N_I-1}}}{dt} = & G_{I_{N_I-1}} + \alpha_{N_I}^- C_{I_{N_I}} + \alpha_{N_I-2}^+ C_I C_{I_{N_I-2}} + k_{I_{N_I-2}-V}^- C_{I_{N_I-2}} - \alpha_{N_I-1}^+ C_I C_{I_{N_I-1}} - \alpha_{N_I-1}^- C_{I_{N_I-1}} - k_{I_{N_I-1}+V}^+ C_V C_{I_{N_I-1}} \\ & + k_{I_{N_I}+V}^+ C_V C_{I_{N_I}} - k_{I_{N_I-1}-V}^- C_{I_{N_I-1}}, \end{aligned} \quad (16)$$

$$\frac{dC_{I_{N_I}}}{dt} = G_{I_{N_I}} + \alpha_{N_I-1}^+ C_I C_{I_{N_I-1}} + k_{I_{N_I-1}-V}^- C_{I_{N_I-1}} - \alpha_{N_I}^- C_{I_{N_I}} - k_{I_{N_I}+V}^+ C_V C_{I_{N_I}}, \quad (17)$$

$$\begin{aligned} \frac{dC_V}{dt} = & G_V + 2\gamma_2^- C_{V_2} + k_{V_2+I}^+ C_{V_2} C_I + \sum_{n=3}^{N_V} \gamma_n^- C_{V_n} + \sum_{n=2}^{N_I+1} k_{I_{n-1}-V}^- C_{I_{n-1}} - k_{I+V}^+ (C_I C_V - C_I^{eq} C_V^{eq}) \\ & - 2\gamma_1^+ C_V^2 - \sum_{n=2}^{N_V} \gamma_n^+ C_V C_{V_n} - \sum_{n=2}^{N_I} k_{I_n+V}^+ C_V C_{I_n} - (k_{D+V}^+ + k_{S+V}^+) C_V, \end{aligned} \quad (18)$$

$$\frac{dC_{V_n}}{dt} = G_{V_n} + k_{V_{n+I}}^+ C_I C_{V_{n+1}} + \gamma_{n+1}^- C_{V_{n+1}} - k_{V_n+I}^+ C_I C_{V_n} + \gamma_{n-1}^+ C_V C_{V_{n-1}} - \gamma_n^- C_{V_n} - \gamma_n^+ C_V C_{V_n}, \quad \text{for } \$2 \leq n \leq N_V - 2, \$ \quad (19)$$

$$\frac{dC_{V_{N_V-1}}}{dt} = G_{V_{N_V-1}} + k_{V_{N_V}+I}^+ C_I C_{V_{N_V}} + \gamma_{N_V}^- C_{V_{N_V}} + \gamma_{N_V-2}^+ C_V C_{V_{N_V-2}} - k_{V_{N_V-1}+I}^+ C_I C_{V_{N_V-1}} - \gamma_{N_V-1}^- C_{V_{N_V-1}} - \gamma_{N_V-1}^+ C_V C_{V_{N_V-1}}, \quad (20)$$

$$\frac{dC_{V_{N_V}}}{dt} = G_{V_{N_V}} + \gamma_{N_V-1}^+ C_V C_{V_{N_V-1}} - k_{V_{N_V}+I}^+ C_I C_{V_{N_V}} - \gamma_{N_V}^- C_{V_{N_V}}. \quad (21)$$

$$\frac{d\rho}{dt} = 2\pi v_{cl} S_{BH} - \rho \tau_{cl}^{-1}. \quad (22)$$

For each defect size and type, a separate evolution equation exists, so that there are $N_I + N_V + 1$ equations in total. Here, the G -terms are for defect production, and the $+$ and $-$ terms are for absorption and emission; C_{I_n} and C_{V_n} are the concentrations of the clusters I_n and V_n respectively, ρ is the dislocation density, v_{cl} is the dislocation climb velocity, S_{BH} is the Bardeen-Herring source density and τ_{cl} is the average network dislocation lifetime prior to dipole annihilation. The individual terms that appear in these equations are given below.

A.1. Defect production

The production rate of SIA- and vacancy defects of size n is modelled with $G_n = G_{n0} \eta (1 - f_D / f_{\max})$ and the power law $G_{n0} = \frac{A_\epsilon}{n^{S_\epsilon}}$ (Mannheim et al., 2019b). Here, ϵ stands for I or V , η is a parameter that expresses the fraction of defects, out of those that survived the thermal aging of the displacement cascade in MD-simulations, that are still present on a cluster dynamics time scale, where $\eta = 1$ is taken here (Mannheim et al., 2019b). Furthermore, f_D is the fraction of atomic sites that contain defects, $f_{\max}$ is the saturated defect fraction level, where $f_{\max} = 0.01$ is used here (Mannheim et al., 2019b), G_0 is the production rate of defects in defect-free tungsten and $A_\epsilon = G_0 / \sum_{n=1}^{N_{\max}} n^{1-S_\epsilon}$, where $N_{\max}$ is the maximum defect size that is accounted for. The parameters G_0 , S_I and S_V are temperature-dependent. Linear interpolation of the values given in Table 2 is used.

Table 2

The defect production rate G_0 and power law exponents S_I and S_V at different temperatures, from Mannheim et al. (2018), based on MD-results (Setyawan et al. (2015)).

T (K)	G_0 (# defects/atom s)	S_I	S_V
300	4.3×10^{-8}	2.20	1.63
1025	3.3×10^{-8}	2.50	1.86
2050	3.1×10^{-8}	2.17	2.42

Table 3

Rate coefficients for defect absorption and emission at clusters, from Li et al. (2012).

Dislocation loop I_n		
Absorption rate	Emission rate	
$\alpha_n^+ = 2\pi r_{I_n} Z_{I_n}^I D_I$	$\alpha_n^- = 2\pi r_{I_{n-1}} Z_{I_{n-1}}^I D_I \exp(-E_{I_{n-1}}^b/k_B T)/V_{at}$	Interstitial
$k_{I_n+V}^+ = 2\pi r_{I_n} Z_{I_n}^V D_V$	$k_{I_{n-1}-V}^- = 2\pi r_{I_{n-1}} Z_{I_{n-1}}^V D_V \exp(-E_{I_{n-1}-V}^b/k_B T)/V_{at}$	Vacancy
$k_{I_n+V}^+ = 4\pi r_{IV} (D_I + D_V)$		VI-recombination
Vacancy cluster V_n		
Absorption rate	Emission rate	
$k_{V_n+I}^+ = 4\pi r_{V_n} D_I$	–	Interstitial
$\gamma_n^+ = 4\pi r_{V_n} D_V$	$\gamma_n^- = 4\pi r_{V_{n-1}} D_V \exp(-E_{V_{n-1}-V}^b/k_B T)/V_{at}$	Vacancy

Although $\eta = 1$ is used in the simulation results that are presented in this paper, it has been verified that by using $\eta = 0.01$ similar results are obtained, and the same physical phenomena play a role (at different time scales).

A.2. Absorption and emission coefficients at defect clusters

The absorption and emission rates of the mobile vacancies and interstitials at/from SIA-clusters and vacancy clusters are given in Table 3 (Li et al., 2012). These rates depend on the capture radii $r_{I_n} = \sqrt{\frac{nV_{at}}{\pi b}}$, and $r_{V_n} = (3nV_{at}/4\pi)^{1/3} + \sqrt{3}a_0/4$ of the I_n (planar shaped) and V_n (spherically shaped) clusters, and on the diffusion coefficients $D_\epsilon = D_{\epsilon_0} \exp(-E_\epsilon^m/k_B T)$ of mobile defects $\epsilon = I, V$. Furthermore, bias factors Z and binding energies are involved, which are detailed below. Lastly, T is the temperature, a_0 is the lattice parameter, V_{at} is the atomic volume, k_B is the Boltzmann constant. The parameter values are given in Table 5.

The binding energies follow from the capillarity approximation (Li et al., 2012):

$$E_{I_n}^f = E_{I_{n-1}}^f + E_I^f - E_{I_{n-1}}^b \text{ (by definition),} \quad (23)$$

$$E_{I_{n-1}}^b = E_I^f + \frac{E_{I_2}^b - E_I^f}{2^{2/3} - 1} [n^{2/3} - (n-1)^{2/3}], \quad (24)$$

$$E_{I_n-V}^b = E_V^f + \frac{E_{I_2}^f - E_{I_2}^b}{2^{2/3} - 1} [n^{2/3} - (n-1)^{2/3}], \quad (25)$$

$$E_{V_{n-1}-V}^b = E_V^f + \frac{E_{V_2}^b - E_V^f}{2^{2/3} - 1} [n^{2/3} - (n-1)^{2/3}]. \quad (26)$$

Here, $E_{I_{n-1}}^b$ is the binding energy of a SIA-defect to a SIA-cluster of size n , and analogous for the other terms. $E_{I_n}^f$ is the formation energy of defect I_n .

The dislocation bias factors (for preferential absorption of SIAs) are given by:

$$Z_{I_n}^I = Z_D^I \max\left(\frac{2\pi}{\ln(8r_{I_n}/r_p)}, 1\right), \quad (27)$$

$$Z_{I_n}^V = Z_D^V \max\left(\frac{2\pi}{\ln(8r_{I_n}/r_p)}, 1\right). \quad (28)$$

Here, $r_p = 2b$ is taken, after (Li et al., 2012).

A.3. Absorption coefficients at grain boundary and dislocation sinks

The absorption rate coefficients of the sinks (Li et al., 2012) are given in Table 4.

Here, r_g is the grain radius and S_I^{sk} and S_V^{sk} are the sums of the sink strengths of all sinks in the interior of the grain:

$$(S_I^{sk})^2 = \frac{1}{D_I} \left[\sum_{n=1}^{N_I-1} \alpha_n^+ C_{I_n} + \sum_{n=1}^{N_V} k_{V_n+I}^+ C_{V_n} \right] + \rho Z_D^I, \quad (29)$$

$$(S_V^{sk})^2 = \frac{1}{D_V} \left[\sum_{n=1}^{N_V-1} \gamma_n^+ C_{V_n} + \sum_{n=1}^{N_I} k_{I_n+V}^+ C_{I_n} \right] + \rho Z_D^V. \quad (30)$$

Table 4

Rate coefficients of the sinks (Li et al., 2012).

Dislocation sink (ρ_D)	
$k_{D+I}^+ = \rho_D^I D_I$	Interstitial
$k_{D+V}^+ = \rho_D^V D_V$	Vacancy
Grain boundary sink	
$k_{S+I}^+ = 3S_g^I D_I / r_g$	Interstitial
$k_{S+V}^+ = 3S_g^V D_V / r_g$	Vacancy

Table 5

Parameter values.

Parameter	Unit	Value	Description	Reference
a_0	nm	0.31652	Lattice parameter	Lassner and Schubert (2012)
γ_b	J/m ²	0.869	GB-surface energy	Lopez (2015)
δ	nm	1	grain boundary thickness	Favre et al. (2013)
D_0^{GB}	m ² /s	0.27×10^{-4}	Self-diffusivity along grain boundaries	Estimated, using Lassner and Schubert (1999)
D_{I_0}	m ² /s	8.77×10^{-8}	SIA-diffusivity	Faney (2013)
D_{V_0}	m ² /s	177×10^{-8}	Vacancy diffusivity	Faney (2013)
E_I^f	eV	9.466	Formation energy SIA	Li et al. (2012)
E_V^f	eV	3.80	Formation energy vacancy	Li et al. (2012)
$E_{I_2}^b$	eV	2.12	Binding energy SIA-SIA	Li et al. (2012)
$E_{V_2}^b$	eV	0.6559	Binding energy V-V	Li et al. (2012)
E_I^m	eV	0.013	SIA migration energy	Faney (2013)
E_V^m	eV	1.66	Vacancy migration energy	Faney (2013)
K_d^A	–	5×10^7	Nucleation activation energy reduction	–
K_m	–	1490	Grain boundary mobility parameter	–
K_N	#/m ² s	2.5×10^{17}	Nucleation rate constant	–
M	–	3.06	Taylor factor	Stoller and Zinkle (2000)
μ	Pa	161×10^9	Shear modulus	Lassner and Schubert (1999)
N_{max}	–	100	Maximum cluster size	–
P_1	–	0.3258	–	Hust and Landford (1984)
P_2	–	2.449	–	Hust and Landford (1984)
P_3	–	147.1	–	Hust and Landford (1984)
P_4	–	-0.22	–	Hust and Landford (1984)
P_5	–	0.1855	–	Hust and Landford (1984)
P_6	–	3.986	–	Hust and Landford (1984)
P_7	–	0.1	–	Hust and Landford (1984)
Q^{GB}	J/mol	4×10^5	Activation energy for GB mobility	Lassner and Schubert (1999)
r_{IV}	nm	0.465	Recombination radius	Li et al. (2012)
Threshold HD-set	J/m ³	1×10^6	–	–
T_{ref}	K	373	Reference temperature	–
V_m	m ³ /mol	9.55×10^{-6}	Molar volume	–
Z_D^I	–	1.2	SIA-dislocation bias	Li et al. (2012)
Z_D^V	–	1	V-dislocation bias	Li et al. (2012)

A.4. Dislocation evolution expressions

In Eq. (22), the evolution of the dislocation density depends on the dislocation climb velocity v_{cl} , which governs dipole annihilation and the Bardeen–Herring source dislocation generation rate, is given by Stoller (1990):

$$v_{cl} = \frac{2\pi}{b \ln R/r_c} [Z_D^I D_I C_I - Z_D^V D_V (C_V - C_V^D)]. \quad (31)$$

Here, $C_V^D = C_V^{eq} \exp(\frac{\sigma V_{at}}{k_B T})$ (Was, 2007) is the equilibrium concentration of vacancies near a dislocation, C_V^{eq} is the equilibrium vacancy concentration in the bulk and $\sigma = A\mu b\sqrt{\rho_p}$ is the internal stress due to pinned dislocations, with a pinned dislocation density $\rho_p = 0.1\rho$; μ is the shear strength, b the Burgers vector magnitude and $A = 0.4$. R/r_c is taken as 2π (Li et al., 2012).

Furthermore, in Eq. (22), the Bardeen–Herring source density is given by $S_{BH} = (\rho_p/3)^{1.5}$ and $d_{cl} = v_{cl} \times \tau_{cl} = (\pi\rho)^{-1/2}$ is the average climb distance for a dislocation prior to annihilation (Stoller, 1990).

Appendix B. Recrystallization model

B.1. Mean-field approach

The representative grains constituting the microstructure at a certain material point, are distributed among the N_{HEM} homogeneous equivalent media (HEMs) based on their bulk stored energies. The stored energy of a grain k with radius $r_{g,k}$ and defect concentrations $C_{ln,k}$ and $C_{Vn,k}$ and dislocation density ρ_k is given by:

$$E_k = E_k^B + E_k^S = \sum_{n=1}^{N_{max}} [C_{ln,k} E_{ln}^f + C_{Vn,k} E_{Vn}^f] + \mu b^2 \rho_k / 2 - TS_k + 3\gamma_b / 2r_{g,k}, \quad (32)$$

where the latter term is the surface stored energy, with γ_b the grain boundary surface energy and the other terms represent the bulk stored energy, E_{ln}^f and E_{Vn}^f are the defect formation energies and S_k is the configurational entropy.

To limit computational costs, there is a maximum amount of representative grains that can exist within each HEM. In case that this amount is about to be exceeded, the two representative grains within the HEM that resemble each other most (in terms of grain size and defect densities) are merged to form one representative grain.

B.2. Grain growth

During grain growth, the grain boundaries move, which leads to shrinkage and growth of the representative grains. The grains are assumed to be of a spherical shape, so the new radius of a grain follows directly from the volume change in a time increment. The volume change ΔV_k of a grain k during a time step $\Delta t = t_{i+1} - t_i$ is given by:

$$\Delta V_k = \sum_{q=1}^{N_{HEM}} \Delta V_k^q = \sum_{q=1}^{N_{HEM}} \phi^q 4\pi r_{g,k}^2 v_{g,k}^q \Delta t = \sum_{q=1}^{N_{HEM}} \phi^q 4\pi r_{g,k}^2 m(E_q^{HEM} - E_k) \Delta t, \quad (33)$$

where $v_{g,k}^q$ is the velocity of the grain boundary segment that is shared between grain k and HEM q , $\phi^q = \sum_{k \in q} N_k r_{g,k}^2 / \sum_{k \in q} N_k r_{g,k}^2$ is the fraction of the grain boundary surface area that HEM q shares with any of the representative grains, E_q^{HEM} is the stored energy of HEM q , E_k is the stored energy of grain k and $m(T) = K_m \frac{\beta \delta V_m}{b^2 R T} D_0^{GB} \exp(-\frac{Q^{GB}}{k_B T})$ is the grain boundary mobility, with V_m the molar volume, δ the thickness of the grain boundary, $\beta = 0.3$ a fraction parameter, Q^{GB} the activation energy for self-diffusion of tungsten along a grain boundary, R the gas constant and D_0^{GB} the self-diffusivity for tungsten along grain boundaries. Grain growth is driven by the difference in stored energy of the HEMs with the grain. The stored energy of a HEM, E_q^{HEM} , is the volume average of the stored energy of its composing grains. The volume that is added to the growing grains is assumed to be defect-free, as the grain boundaries sweep the defects on their path. The new defect concentration of a grain k to which a defect-free volume ΔV_k^{growth} was added in increment $\Delta t = t_{i+1} - t_i$ is given by:

$$C(t_{i+1}) = C(t_i) - \frac{\Delta V_k^{growth}}{V_k(t_{i+1})} [C(t_i) - C^{eq}]. \quad (34)$$

Here, $C(t)$ is the defect concentration at time t , $V_k(t)$ is the volume of the grain at time t and C^{eq} is the equilibrium defect concentration.

For reasons of volume conservation, the shrinkage of grains with respect to their own HEM is calculated in an alternative manner (based on Bernard et al., 2011):

$$\Delta V_k^q = -4\pi m \Delta t r_{g,k}^2 \phi^q \Delta E_k \frac{\sum_{k \in q: \Delta V_k^q > 0} \Delta V_k^q N_k}{\sum_{k \in q: \Delta V_k^q < 0} \Delta V_k^q N_k}, \quad (35)$$

where ΔV_k^q denotes the volume change of a grain k as a consequence of the interaction with HEM q .

B.3. Nucleation

Driven by the stored lattice energy, defect-free nuclei form. The nucleation rate is given by:

$$\dot{N} = K_N A_{nuc} \exp\left(\frac{-E_{act}}{k_B T}\right) \exp\left(\frac{-Q^{GB}}{k_B T}\right), \quad (36)$$

where K_N is the nucleation rate constant, A_{nuc} is the nucleation surface area and E_{act} is the activation energy. The nucleation radius is found from solving: $d\Delta E/dt < 0$, which is the condition for a stable new grain. ΔE is the Gibbs free energy change as a consequence of the nucleation, which is given by:

$$\Delta E = \frac{1}{K_a} \left[-\frac{4\pi r^3}{3} (E^B - E_0^B) + 3\pi r^2 \gamma_b \right]. \quad (37)$$

Here, K_a is a fitting parameter (Mannheim et al., 2019b), $E^B = \sum_{q=1}^{N_{HEM}} \phi^q E^q$ is the average bulk stored energy and E_0^B is the bulk stored energy for a grain with equilibrium defect concentrations. From Eq. (37), it follows that

$$\frac{d\Delta E}{dt} = \frac{\partial \Delta E}{\partial r} \frac{dr}{dt} + \frac{\partial \Delta E}{\partial E^B} \frac{dE^B}{dt} < 0, \quad (38)$$

is solved. Here, dE^B/dt is determined numerically. Finally, the radius of the nucleus is taken as $r_{nuc} = 1.01r_0$, with r_0 the largest of the solutions to Eq. (38), and the activation energy is $E_{act} = \Delta E(r^*)$, where r^* is the solution of $d\Delta E/dr = 0$.

The nucleation surface area consists of all grain boundary surface area in the microstructure, except for the grain boundary segments that are shared between two grains that have bulk stored energies below the nucleation threshold $E_{nuc}^{B,thr}$:

$$A_{nuc} = 2\pi \sum_i r_i^2 N_i \left[1 - \left(\frac{\sum_{j: E_j < E_{nuc}^{B,thr}} N_j r_j^2}{\sum_j N_j r_j^2} \right)^2 \right]. \quad (39)$$

In this mean-field approach, the volume of the nucleated grains is delivered by all the grains in the microstructure, weighted with their grain boundary surface areas.

Appendix C. Parameter values

The empirical function W_c of Eq. (6) is given by:

$$\begin{aligned} W_c = & -0.0085 \ln\left(\frac{T}{130}\right) \exp\left[-\left[\frac{1}{0.7} \ln\left(\frac{T}{230}\right)\right]^2\right] \\ & + 0.00015 \exp\left[-\left[\frac{1}{0.8} \ln\left(\frac{T}{3500}\right)\right]^2\right] \\ & + 0.0006 \ln\left(\frac{T}{90}\right) \exp\left[-\left[\frac{1}{0.4} \ln\left(\frac{T}{80}\right)\right]^2\right] \\ & + 0.0003 \ln\left(\frac{T}{24}\right) \exp\left[-\left[\frac{1}{0.5} \ln\left(\frac{T}{33}\right)\right]^2\right]. \end{aligned} \quad (40)$$

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