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Citation for published version (APA):
Shah, V., van Dommelen, J. A. W., Heijkoop, S. E. S., Oude Vrielink, M. A., & Geers, M. G. D. (2021). A numerical model for the recrystallization kinetics of tungsten monoblocks under cyclic heat loads. Fusion Engineering and Design, 173, [112827]. https://doi.org/10.1016/j.fusengdes.2021.112827

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DOI:
10.1016/j.fusengdes.2021.112827

Document status and date:
Published: 01/12/2021

Document Version:
Publisher’s PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
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A numerical model for the recrystallization kinetics of tungsten monoblocks under cyclic heat loads

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ARTICLE INFO

Keywords:
Tungsten
Cyclic heat load
Finite element model
Recrystallization
JMAK Model

ABSTRACT

The recrystallization assisted microstructural changes during cyclic heat exposure are surmised detrimental to the thermal fatigue resistance of the tungsten monoblocks that cover the surface of the divertor components of a nuclear fusion reactor. A numerical framework to predict recrystallization in tungsten monoblocks during cyclic heat exposure is presented in this work. The framework is based on a thermal model coupled to a Johnson-Mehl-Avrami-Kolomogorov (JMAK) type recrystallization model. The influence of the initial (starting) microstructural state, i.e. the degree of deformation, on the extent of recrystallization, is considered through the activation energy for recrystallization. For a highly deformed microstructure, significantly more recrystallization is observed compared to self-diffusion driven recrystallization. The activation energy for recrystallization within the range 322 to 350 kJmol$^{-1}$ during cyclic heat exposure of a monoblock is determined from the simulated recrystallization extent in relation to the experimental observations of differently processed monoblocks. The influence of the heating time per cycle for different activation energies on the recrystallization extent is also investigated. Instead of bulk recrystallization, only localized surface recrystallization is observed for a combination of a shorter heating time per cycle and a moderately deformed initial microstructure, which may contribute to improving the thermal fatigue resistance of the monoblocks.

1. Introduction

The viability of fusion reactors as a sustainable and commercial source of energy necessitates a prolonged lifetime of their components. In future tokamak based reactors such as ITER and DEMO, the plasma facing components (PFCs) of the divertor, located at the bottom of the vessel, are regarded as some of the most vital components, as they extract heat from the plasma, simultaneously serving as an exhaust for helium ions as well as plasma impurities [1,2]. Hence, they are subjected to extreme cyclic heat loads and particle loads in the form of ions and neutrons [3,4]. The PFCs are made of bcc metal tungsten (W), due to its wide operating temperature range, in addition to its high thermal conductivity, and plasma compatibility [5]. In case of ITER, these W PFCs consist of an array of actively cooled monoblocks, with a W tile brazed to a CuCrZr alloy tube, thereby resulting in a steep temperature gradient in the monoblock with values that remain within the safe operating range during steady-state operation (10 MWm$^{-2}$) [6]. However, during operation, additional cyclic heat loads in the form of slow transients (20 MWm$^{-2}$, max. 10 s; also qualify as steady-state loads) and fast transients (1–60 MWm$^{-2}$, 0.1–300 ms) will occur, ultimately increasing the temperature, and the magnitude of the associated gradient in the monoblock [6–8].

In experimental studies, the influence of such cyclic heat loads is simulated via laser, plasma and/or electron beam exposure, and several surface based damage mechanisms such as melting, erosion, roughening, and crack-formation under steady-state heat loads are observed, along with an increase in the severity for transients [9–16]. Furthermore, taking into account the actual monoblock geometry and the temperature gradient (reactor like), dedicated long term cyclic high heat flux (HHF) exposure studies have investigated the thermal fatigue resistance of the monoblocks [17–24]. In these studies, the performance of these monoblocks has been investigated with respect to different loading schemes (number of cycles and electron beam diameter), joining technologies between the W-CuCrZr tube, and microstructural orientation. The most commonly reported phenomenon in these studies is macro-crack formation, also known as self-castellation of monoblocks, with deep cracks extending into the bulk of the monoblocks [17–19, 21–23]. Apart from the macro-cracks, pronounced microstructural

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https://doi.org/10.1016/j.fusengdes.2021.112827
Received 23 February 2021; Received in revised form 1 July 2021; Accepted 29 July 2021
Available online 17 August 2021
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changes due to high temperature assisted recrystallization and grain growth are typically observed in the top part of the monoblocks (high temperature regions), with varying fractions in the bulk, depending on the monoblock geometry and loading scheme [14,16,18,21,23].

The macro-crack formation during HHF exposure has been linked to tungsten’s brittleness in the recrystallized state, thereby leading to crack-nucleation at the surface, followed by crack-growth in the bulk due to tensile stresses during cooling [25]. Furthermore, this brittle behaviour of recrystallized tungsten, implying a higher brittle-to-ductile transition temperature (BDTT) is attributed to segregation of impurities and the associated weakening of the grain boundaries (predominantly high angle grain boundaries) [26,27]. Nevertheless, relatively better ductility of recrystallized tungsten (compared to deformed state) has been reported by several studies, thereby suggesting a lower BDTT [28–31]. In terms of macro-crack formation, exhaustion of the ductility of recrystallized tungsten has also been suspected as the underlying cause of macro-crack formation during the HHF exposure [23,32]. For failure predictions of the monoblock, i.e. the number of cycles to crack formation, the influence of recrystallization on mechanical property such as the change in yield stress, and the resulting incremental increase in the plastic strain during cyclic loading is accounted for in infinite element models [25,30,32,33]. Different possible recrystallization depths arising from cyclic HHF exposure have been modelled, with larger depths showing the smallest resistance to crack-formation (failure at lower cycles) [25,32,34]. On the other hand, despite the experimentally observed extended recrystallization in the monoblock bulk, no trace of macro-cracks have been observed in monoblocks from different manufacturers such as AT&M China and ALMT Japan (plasma-facing units produced by Ansaldo Nucleare, Italy; Atmostat, France; CNIM, France; or Research Instruments (RI) GmbH, Germany), thereby highlighting the role of processing and tungsten grade [16,19,24]. Thus, the role of recrystallization in affecting the failure behaviour of monoblocks is unclear. It is also worthwhile to mention that the aforementioned observations of recrystallization and macro-crack formation are strongly sensitive to the initial microstructural state of the monoblocks [17,18,23] as well as the monoblock geometry [2]. Furthermore, a single macro-crack may not have detrimental consequences for the monoblock (for example, through the loss of thermal conductivity and/or structural integrity), but this depends on the actual location/magnitude of the crack.

Since the non-equilibrium concentration of defects drives the recrystallization process, i.e. pre-dominantly dislocations in the case of plastic deformation [35], the recrystallization kinetics is known to be strongly dependent on the degree of deformation, and the resulting microstructural features such as defect density and grain size [23,36]. For example, for highly deformed W plates (cold-rolled to some extent), recrystallization is shown to be proceeded by grain boundary diffusion due to the lower spacing between the low angle grain boundaries (short-circuit diffusion paths) [37–39]. In contrast, for lower deformation levels or warm rolled plates, the recrystallization is driven by self-diffusion mechanism, thereby raising its thermal stability [38,40,41]. Thus, to accurately predict the thermo-mechanical behaviour of the monoblocks during long time cyclic HHF exposure, the dynamic evolution of the microstructure due to recrystallization in conjunction with the initial state is necessary. Previously, based on experimental recrystallization kinetics, Durif et al. [42] proposed an inverse methodology to predict the recrystallized fraction in a monoblock following a few cycles of HHF exposure. However, in this work, the dynamic evolution of the recrystallization fraction over time, and the influence of the initial microstructure were not taken into account.

In the present article, a novel numerical approach to account for the evolution of the recrystallized fraction during cyclic HHF loading is proposed, which allows for assessment of the influence of the dynamically changing microstructural state on the thermo-mechanical behaviour (not addressed here). This approach is based on a thermal heat conduction model coupled with a Johnson-Mehl-Avrami-Kolmogorov (JMAK) based recrystallization model. Additionally, by using suitable parameters for the recrystallization kinetics, it is possible to reproduce the experimentally determined recrystallization behaviour in plasma facing components during cyclic HHF exposure. The article is structured in the following manner. In Section 2, the experimental observations of recrystallization in the HHF exposed monoblock are highlighted. In Section 3, the numerical modelling setup of the monoblock geometry and the simulated load cases are detailed. In Section 4, the simulated load case scenarios are presented along with an extensive discussion. Lastly, in Section 5, a brief summary and conclusions drawn from the present work are given.

2. Experimental observations: Recrystallization in a W monoblock

Tungsten monoblocks manufactured via rolling by AT&M, China and exposed to cyclic HHF loads achieved via an electron beam at IDTF (ITER divertor testing facility, Russia) were delivered by Research Instruments (RI) GmbH. The geometry of these monoblocks followed the ITER specifications [6], i.e. a width of 28 mm, axial length of 12 mm, and an armour thickness equal to 8 mm. The monoblocks were diffusion bonded to a Cu interlayer, and were brazed to the CuCrZr alloy cooling tube [24]. For cyclic loading, the HHF exposure of the ITER divertor qualification program was utilized, where the assembly of tungsten monoblocks (also called the mockups) was exposed to 5000 cycles of 10 MWm⁻² and 1000 cycles of 20 MWm⁻² heat load. Each thermal cycle during the exposure consisted of a 10 s heating phase followed by a 10 s cooling phase. It is important to note that an armour thickness of 8 mm, corresponding to the former monoblock geometry [6] has been adopted in the present work for accurately reproducing the experimental observations. At present, the armour thickness has been reduced to 6 mm following the optimization of the ITER divertor design [43].
A full-scale material characterization of these monoblocks was performed by machining and preparing metallographic samples [16]. Fig. 1 shows an optical micrograph from one of the prepared samples. Two different microstructures, i.e., recrystallized near the top and initial at the bottom can be observed. Furthermore, a spatial variation of the extent of recrystallization is also visible in Fig. 1, with regions closer to the cooling tube showing a transition to the initial microstructure at lower depths (line CD) than regions away from the cooling tube (line AB). The microstructural changes due to recrystallization shown in Fig. 1 were further confirmed by performing hardness measurements (see Fig. 11 in Appendix A), with a lower hardness for the recrystallized area due to its lower defect density.

The aforementioned experimental observations on the extent of recrystallization in the heat exposed monoblocks are reproduced to assess the validity of the numerical model. This then allows to gain insights into the driving mechanism of recrystallization and its dependency on the initial microstructural state.

3. Material monoblock models and solution methodology

In this section, the geometry, boundary conditions, and material properties of the finite element based monoblock model are described, along with its coupling to the JMAK model for evaluating the temperature-dependent recrystallized fraction in the monoblock.

3.1. Thermal monoblock model

Following the experimental observations, the modelled monoblock geometry consists of a W monoblock as the armour material, along with a copper-chromium-zirconium (CuCrZr) cooling tube running through the monoblock as the heat sink. Moreover, to compensate for the thermal expansion mismatch, a copper (Cu) interlayer is placed between the monoblock and its coupling to the JMAK model for evaluating the properties of the finite element based monoblock model are described, along with the modelled one. For discretizing the geometry, the commercial finite element analysis code MSC.Marc is used. Following a mesh-sensitivity analysis and in view of computational efficiency for simulating a large number of cycles, the model is meshed with 5624 eight node isoparametric brick elements.

The thermal behaviour of the monoblock during cyclic HHF exposure is simulated by implicitly solving the conventional transient heat conduction equation, with a global step size of 1 s. The use of a rather coarse global time step is necessary for the computational feasibility, given the large number of cycles and the marginal differences between the full recrystallized depth at the end of heating cycles (5 or 10 s). The evolution of the recrystallized fraction within one heating cycle is simulated using a global step size of 0.1 s, to accurately track the evolution at shorter time scales. At the monoblock surface, a heat flux based boundary condition is prescribed (Fig. 2b). Near the cooling tube, a convection based cooling boundary condition representing the cooling water is employed (Fig. 2b). The convection based boundary condition contains contributions from two different mechanisms, i.e., forced convection due to pressurized flowing water and boiling cooling. For forced convection, a Sieder/Tate correlation is used [44], and for cooling through boiling, the Thom/CEA correlation is used [45]. Based on the above relations, the heat transfer coefficient \( h_{bt} \) is computed from the total heat flux \( q_{bt} \), i.e., \( h_{bt} = \frac{q_{bt}}{T_{w} - T_b} \), where \( T_w \) and \( T_b \) are the wall and bulk fluid temperature. Considering a bulk fluid temperature \( T_b \) equal to 100 \(^\circ\)C, a fluid pressure equal to 3.3 MPa and a fluid velocity equal to 10 ms\(^{-1}\), a wall temperature \( T_w \) dependent heat transfer coefficient \( h_{bt} \) between 70 to 230 kWm\(^{-2}\)K\(^{-1}\) (for temperature range: 50\(^\circ\)C to 230\(^\circ\)C) is used, consistent with values reported by Li and You [25].

To simulate the experimental conditions, a heat load of 20 MWm\(^{-2}\) is applied for thousand cycles (lower number of cycles are also simulated in some cases), with a heating phase lasting for 10 s followed by a cooling phase of 10 s, i.e., in total 20 s per cycle. Also, for all simulations, a homogeneous temperature initial condition of 200\(^\circ\)C is prescribed in the entire monoblock. Contrary to experiments, the lower surface heat load, i.e., 10 MWm\(^{-2}\) is not considered, since it entails an overall lower magnitude of temperature in the monoblock than for the 20 MWm\(^{-2}\) case, thereby predominantly resulting in microstructural changes near the surface only.

Since the 20 MWm\(^{-2}\) HHF exposure of the monoblocks results in a wide temperature range in the monoblock, a temperature dependency of the material properties, i.e., the thermal conductivity \( \kappa \), and the product of mass density and the specific heat \( \rho C \) are adopted for the W, Cu and CuCrZr alloy. The temperature dependent behaviour of these properties for the three different materials are provided in Appendix B. The resulting temperature field in the monoblock after a 10 s exposure to 20 MWm\(^{-2}\) is shown in Fig. 2c, which is in adequate agreement with experimental and numerical observations [24,46].

3.2. Recrystallization model

Recrystallization is a thermally activated process, the extent of which is governed by the exposure time at a given temperature. For isothermal conditions, the kinetics of recrystallization can be described by the JMAK model [47], given as:

\[
X = 1 - \exp\left( B \left( \frac{t}{t_{50}} \right)^n \right)
\]  

(1)

with \( X \) being the recrystallized fraction, \( B \) being a constant (equal to 0.693, considering 50% recrystallization, i.e. \( \ln(0.5) \)), \( n \) representing the Avrami exponent, and \( t_{50} \) representing the time required to achieve 50% recrystallization (time to half recrystallization). Furthermore, taking into account the temperature dependency, the time to half recrystallization \( t_{50} \) can be expressed as:

\[
t_{50} = t_{50}^{\text{act}} \exp\left( \frac{E_{\text{act}}}{RT} \right)
\]

(2)

where, \( t_{50}^{\text{act}} \) is the pre-exponential factor, \( E_{\text{act}} \) is the activation energy for recrystallization, \( R \) is the real gas constant and \( T \) is the annealing temperature. Experimentally, information regarding the recrystallized fraction \( X \) for a given material state can be obtained by performing hardness measurements following annealing at a given temperature. Repeating this over a wide range of temperatures, the above JMAK parameters can be determined. However, under non-isothermal conditions, the temperature governed recrystallized fraction should be modelled using a differential form of the JMAK equation [47]:

\[
\frac{dX}{dt} = 0.693 n \left( \frac{1 - X}{t_{50}} \right) \ln\left( \frac{1}{1 - X} \right) \exp\left( \frac{E_{\text{act}}}{RT} \right)
\]

(3)

In the present work, this differential form of the JMAK model is used to track the temporal evolution of the recrystallized fraction during cyclic HHF exposure of the monoblock. The pre-exponential factor \( t_{50}^{\text{act}} \) for time to half-recrystallization \( t_{50} \) is determined from the experimentally measured time to half recrystallization on annealed rolled tungsten [39, 48], while the activation energy for the recrystallization \( E_{\text{act}} \) is used as an input parameter to account for the degree of prior deformation. Based on the results from the experimental annealing studies [38,39], a constant Avrami exponent \( n \) equal to 2 is used for all simulations. Note that a
temperature dependence of the Avrami exponent $n$, as suggested in experimental studies was also simulated [41,49], but its influence on the recrystallization behaviour of the monoblock was shown to be insignificant.

3.3. Coupled solution procedure

The temperature-dependent recrystallized fraction is calculated within the finite element based thermal monoblock model using a subroutine implemented in MSC.Marc. Here, for each global time step of the monoblock thermal problem, the subroutine is invoked at the integration points, with the temperature and recrystallized fraction (from previous time step) serving as input for the subroutine. The updated recrystallized fraction within the subroutine is calculated by discretizing the JMAK differential (eq. (3)) explicitly in time, i.e. using Forward Euler. Here, a constant time step with a relatively small step size of $2.5 \times 10^{-4}$ s (local time step) is used to ensure the stability of the solution along with computational efficiency. For the initial condition, the recrystallized fraction in the entire monoblock is set equal to 0.001, corresponding to a deformed starting state.

3.4. Simulated cases

For assessing the extent of recrystallization in the monoblock during cyclic HHF exposure, two different cases related to the input JMAK parameter and exposure time are investigated. First, the recrystallization in the monoblock is explored as a function of the initial microstructural state, i.e. the starting state. Here, the dependency of the JMAK parameter, i.e. the activation energy for recrystallization $E_{\text{act}}$, on the degree of deformation is taken into account following experimental observations [38–41]. Secondly, the influence of a shorter exposure (heating) time, i.e. 5 s, on the recrystallization extent is explored for different activation energies and compared to the standard case of 10 s exposure per cycle.

4. Results and discussion

In this section, the simulated recrystallization behaviour of the monoblock during cyclic HHF exposure is presented, and discussed in terms of the input activation energy, and the exposure time per cycle.

4.1. Recrystallization behaviour in the monoblock

The evolution of the recrystallized fraction in the monoblock during high heat load exposure between the points C and D (Fig. 2b) of the monoblock and for an activation energy of 300 kJmol$^{-1}$ is shown in Fig. 3. The results for this case are detailed specifically due to its relevance to the experimental observations, thereby providing profound insights on the cycle dependent evolution. In Fig. 3a, the evolution of the recrystallized fraction within a single cycle is shown, where the extremely high temperatures resulting from the heat exposure almost instantly lead to full recrystallization of the regions near the surface, i.e. within 3 s, with full recrystallization up to a depth of 1.4 mm. Moreover, as the exposure progresses, the recrystallization front moves to the monoblock bulk, ultimately leading to a full recrystallization depth of approximately 3.4 mm at the end of the 10 s exposure cycle.

In Fig. 3b, the evolution of the recrystallized fraction as a function of the number of cycles is shown. Initially, for time scales corresponding to few tens of cycles, the recrystallization front moves steadily along the bulk (nearly equal distance between the recrystallization fraction trend lines at $X = 0.5$), whereby the fully recrystallized region grows from 4 mm to 4.5 mm between 10 to 32 cycles. This expanding trend for the fully recrystallized region continues up to a depth of 5.2 mm after 316 cycles. However, at longer time scales such as the ones between 316 to

![Fig. 2. Geometry of the water cooled tungsten monoblock considered for the numerical model in the present work (a); FE discretization and boundary conditions (b); the resulting temperature field in the monoblock at the end of a 10 s exposure cycle for 20 MWm$^{-2}$ surface heat load (c).](image-url)
1000 cycles, the recrystallization progress reduces drastically due to the relatively lower temperatures in the bulk monoblock, thereby necessitating longer times for full recrystallization. Nonetheless, at longer time scales, i.e. between 316 to 1000 cycles, a small propagation of the recrystallization front towards larger depths persists.

The influence of the starting microstructural state on the recrystallized fraction is compared in Fig. 4 by plotting the recrystallized fraction evolution for different activation energies. In Fig. 4a, the evolution after 300 cycles is shown while in Fig. 4b, the evolution after 1000 cycles is depicted. A significant dependency of the recrystallized fraction on the activation energy can be observed in both figures, with overall a lower activated fraction is compared in Fig. 4 by plotting the recrystallized fraction on the activation energy can be related to the thermally activated process. However, for nucleation, the role of grain boundaries as the rate controlling process is only applicable when the nucleation mechanism is considered to be governed by subgrain growth [35].

For further insights into the evolution of the fully recrystallized fraction in the monoblock, Fig. 5a compares the temporal evolution of the fully recrystallized depth for different activation energies. Here, the data points resemble the fully recrystallized depth after certain exposure time, including the cooling cycles. Considering the lowest activation energy case, i.e. 300 kJmol$^{-1}$ as an example, the exposure time-dependent fully recrystallized region in the monoblock expands at a constant rate with the exposure time. A similar expanding trend with exposure time is also visible for other activation energies, whereby the overall recrystallized depth is smaller for an increasing activation energy. This overall decreasing recrystallization depth with increasing activation energy (irrespective of the exposure time) is due to the time to half recrystallization ($X = 50\%$) between the points C and D (Fig. 2b) of the monoblock, evaluated using the steady state-temperature profile at the end of a 10 s exposure.

Apart from the evolution of the recrystallized fraction in the regions

![Fig. 4. The recrystallized fraction evolution in tungsten monoblock (between points C and D in Fig. 2b) for different activation energies in kJmol$^{-1}$ after 300 cycles (a) and 1000 cycles (b) during 20 MWm$^{-2}$ heat load exposure. For highly deformed initial state, the extent of recrystallization in the monoblock evolves primarily during the first few hundred exposure cycles, and progresses slowly for longer exposure time. On the other hand, for low to moderately deformed initial microstructure, independent of the number of exposure cycles, the extent of recrystallization in the monoblock is minimal.]

![Fig. 5. Temporal evolution of the fully recrystallized fraction between the points C and D (Fig. 2b) of the monoblock for different activation energies (a). The exposure time indicated in the figure corresponds to a sequence of heating and cooling cycles. (b) The activation energy and depth (temperature) dependent time to half recrystallization ($X = 50\%$) between the points C and D (Fig. 2b) of the monoblock, evaluated using the steady state-temperature profile at the end of a 10 s exposure.](image-url)
near the cooling tube (point C and D in Fig. 2 b), the regions farther away from the cooling tube experience relatively high temperatures (as seen in Fig. 2 b), thereby resulting in a larger extent of recrystallization. This is depicted in Fig. 6 showing two-dimensional contour maps of the recrystallized fraction in the monoblock following 1000 exposure cycles with different activation energies. The extent of recrystallization increases with increasing distance from the cooling tube, thereby accurately reproducing the experimentally observed behaviour (Fig. 1).

In terms of the activation energy, the overall extent of recrystallization at any spatial location in the monoblock away from the cooling tube tends to be lower with increasing activation energy.

The recrystallization depth results from the different simulated cases after 1000 exposure cycles were used to construct an activation energy dependent full recrystallization map, as shown in Fig. 7. The data points in this figure represent the simulated fully recrystallized depths for a given activation energy, while the solid lines are the trend lines. For a quantitative comparison, the recrystallization depths along the centre and the edge of the monoblock are shown, and it can be followed from Fig. 7 that with increasing activation energy, the difference between the fully recrystallized region in the centre and at the edge of the monoblock decreases.

Taking into account the experimental observations and using an inverse methodology, this figure can be used to predict the initial microstructural state of the monoblock, for which the prior degree of deformation ($E_{\text{act}}$) and the corresponding recrystallization behaviour is not known. For example, considering the experimental observations on the extent of recrystallization in the heat exposed AT&M monoblock shown in Fig. 1, i.e. a recrystallization depth of approximately 5 mm near the centre and 7 mm near the edge, Fig. 7 provides an activation energy of approximately 322 kJmol$^{-1}$, i.e. within the grain boundary diffusion range. Also, considering the lower number of exposure cycles (300 cycles) and a recrystallization depth of 4 mm in the centre and 5.2 mm at the edge of the heat exposed Plansee AG manufactured (forging) monoblocks (similar geometry) from the work of Nogami et al. [21], results in a similar activation energy of 350 kJmol$^{-1}$, i.e. in the range of grain boundary diffusion (see Appendix C). Nonetheless, it is also

Fig. 6. The recrystallized fraction in the monoblock following 1000 cycles of 10 s exposure with 20 MWm$^{-2}$ heat load for different activation energies ($E_{\text{act}}$) between 300 to 600 kJmol$^{-1}$.

Fig. 7. Activation energy dependent fully recrystallized depths along the centre and edge of the monoblock following 1000 cycles of 10 s exposure for 20 MWm$^{-2}$. As the activation energy for recrystallization increases, the overall recrystallization depth and the difference between the recrystallization fronts between the centre and the edge of the monoblock decreases.

Fig. 8. Temperature field in the monoblock at the end of a 5 s cycle exposure of 20 MWm$^{-2}$ heat load (a) isometric view, with one-dimensional line plot showing the comparison between the temperature gradient between the points C and D of the monoblock (Fig. 2b) at different heating time intervals (b).
important to point out that the evolution of the recrystallized fraction in the monoblock occurs in the presence of stress, which may accelerate the recrystallization process \cite{51,52}. Hence, the activation energy determined by this inverse methodology rather represents a lower bound value. In this context, a measure of the influence of stress on the recrystallization kinetics (not considered here) can be obtained by comparing the activation energy determined from oven annealing experiments with the one predicted by the inverse methodology following experimental high heat exposures of monoblocks.

4.2. Influence of exposure time per cycle

In the standard case highlighted above, the exposure time per cycle was equal to 10 s corresponding to the maximum duration of slow transients (as in the experimental exposure). Yet, shorter duration transitions can also occur \cite{53}. Hence, the influence of shorter exposure times on the recrystallized fraction in the monoblock is investigated by simulating cycles with a lower heating time per cycle, i.e. 5 s instead of 10 s. The temperature field in the monoblock at the end of a single 5 s exposure cycle is shown in Fig. 8a. A lower magnitude of temperature at

Fig. 9. Comparison of the evolution of the fully recrystallized depth (between points C and D) as a function of the accumulated heating time with different heating time per cycle for $E_{\text{act}}$ (a) 350 kJmol$^{-1}$, (b) 450 kJmol$^{-1}$.

Fig. 10. Two dimensional contour plots portraying the recrystallized fraction in the monoblock following 600 cycles of 5 s (a) and 10 s (b) exposure with 20 MWm$^{-2}$ heat load for three different activation energies ($E_{\text{act}}$), i.e. 350 kJmol$^{-1}$, 450 kJmol$^{-1}$, and 550 kJmol$^{-1}$.
the end of 5 s can be observed in the monoblock as compared to the 10 s case (Fig. 2b versus Fig. 8a). This is more clear in Fig. 8b, where the temperature gradient between the points C and D of the monoblock at different time instances are shown. After 5 s exposure, the temperature at point C is nearly 100 °C lower than after 10 s exposure.

To investigate the influence of the exposure time per cycle, the fully recrystallized region in the monoblock for both 5 s and 10 s heating cycles, are represented in Fig. 9 in terms of the accumulated heating time, i.e. the total heating time accumulated over the cycles. As shown in Fig. 9a, i.e. for a lower activation energy of 350 kJ mol\(^{-1}\), considering the accumulated heating time, the 10 s heating cycles lead to a larger fully recrystallized depth than the shorter 5 s heating cycles, independent of the exposure time scale. An identical behaviour of larger recrystallized depth for the 10 s heating cycles (similar accumulated heating time) also emerges for the higher activation energy case, i.e. 450 kJ mol\(^{-1}\) in Fig. 9b, with an overall lower recrystallized depth due to higher activation energy (higher thermal stability; less defect density) independent of the heating time per cycle as observed and reasoned previously. The larger fully recrystallized depth for the 10 s heating cycles compared to the 5 s ones, is likely due to the non- steady-state temperature in the beginning of each heating cycle, as shown in Fig. 8b. Ultimately, this results in a higher recrystallization rate for the 10 s exposure (as per Fig. 5b). Note that for a higher activation energy (corresponding to the self-diffusion mechanism), a similar influence of the exposure time per cycle occurs, i.e. a lower recrystallization depth for shorter heating cycles, but at relatively longer exposure time (not shown here).

In addition to the comparison based on the accumulated heating time, Fig. 10a highlights the influence of shorter exposure cycles, i.e. 5 s heating on the recrystallized fraction in the monoblock after 600 cycles for different activation energies. For comparison, the evolution of the recrystallized fraction for varying activation energies after 600 cycles of 10 s heating per cycle is shown in Fig. 10b. Considering the equivalent number of exposure cycles, from both these figures, it can be observed that independent of the activation energy accounted for, the lower temperature magnitude in the monoblock during a 5 s heating cycle leads to an overall lower recrystallized fraction than for the 10 s heating cycle. Moreover, Fig. 10a also shows that exposure to shorter heating time per cycle combined with an higher activation energy results in minimal recrystallization of the monoblock. This may be beneficial if recrystallization and the associated drop in yield stress impacting ductility are considered detrimental for the monoblock’s high cycle thermal fatigue resistance. However, here two major challenges are foreseen. The first one is related to the microstructural design problem, i.e. e. a microstructural state with a higher activation energy necessitates an overall lower degree of pre-deformation, implying a lower yield strength than the highly deformed microstructural state. The innate consequence of such a microstructure under cyclic HIF exposure will be a higher tendency to undergo plastic deformation. Secondly, the actual fusion conditions entail particle loads, i.e. neutrons and plasma ions, with neutrons having a two-fold influence depending on temperature. Near the monoblock surface, the additional driving force from displacement damage in combination with high temperatures at longer time-scales, may result in a higher recrystallized fraction than the thermal loading only case, as shown by Mannhein et al. [54] through a multi-scale neutron induced recrystallization model (similar to the dynamic recrystallization mechanism). In the bulk regions with lower temperatures, a shift in BDIT to higher temperatures can occur due to the hardening caused by the neutron induced defects, thereby increasing the risk of failure near the cooling tube. Moreover, the helium bubble formation in the high temperature regime of the monoblock [48] could lead to degradation of its thermal conductivity, entailing an increase of the temperature in the sub-surface regime, eventually accelerating the kinetics of recrystallization.

5. Summary and conclusions

A novel modelling framework, coupling transient heat flow to the JMAK model to predict the dynamic evolution of the temperature dependent recrystallized fraction in tungsten monoblocks during cyclic heat exposure is presented. The influence of the initial microstructural state on the extent of recrystallization is accounted through the deformation governed activation energy. Additionally, the sensitivity to the exposure time per cycle is investigated. The main conclusions from this work are summarized below:

- The recrystallization of the monoblock reveals a high sensitivity to the input activation energy. For a highly deformed initial state, i.e. enabling grain boundary diffusion driven recrystallization with a lower activation energy, the extent of recrystallization was notably larger than the moderately deformed microstructural state, driven by self-diffusion with a higher activation energy.
- An activation energy in the range 322 to 350 kJ mol\(^{-1}\) corresponding to grain boundary diffusion driven recrystallization was determined from experimental observations of recrystallization in different cyclic high heat exposed monoblocks using an inverse methodology.
- A significant influence of the exposure time on the recrystallization of the monoblocks was observed. For a given activation energy, the extent of recrystallization was lower for a shorter exposure time than for a longer one. This was due to the development of the overall lower temperature profile in the monoblock, which differs for shorter exposure times relative to the longer ones.
- Localized recrystallization in the monoblocks’ surface was observed for shorter exposure times combined with a moderately deformed starting microstructural state (a higher activation energy). This revealed that the initial state with a low defect density and controlled slow transients could minimize the recrystallization assisted bulk microstructural changes, but at the expense of a lower yield strength.

For future work, the developed thermal recrystallization can be coupled to the mechanical monoblock problem, thereby allowing to gain better insights into the influence of the dynamically evolving micro-structure on the thermo-mechanical performance of the monoblock. Additionally, the evolving thermo-mechanical behaviour under cyclic exposure can be combined with a model for the BDIT of recrystallized tungsten to obtain more accurate monoblock failure predictions. Apart from the monoblock geometry, the developed numerical framework can be used as an engineering tool to predict the dynamically evolving recrystallized fraction and its influence on the mechanical behaviour of components experiencing high temperatures with a strong temperature gradient, which is relevant for the different conceptual future plasma facing component geometries.

Data availability

The raw or analysed data reported in this study are available upon reasonable request.

CRediT authorship contribution statement

V. Shah: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft. J.A.W. van Dommelen: Conceptualization, Funding acquisition, Methodology, Resources, Project administration, Supervision, Writing – review & editing. S.E.S. Heijkoop: Data curation, Formal analysis, Investigation, Methodology, Software, Writing – review & editing. M.A. Oude Vrielink: Investigation, Methodology, Software, Writing – review & editing. M.G.D. Geers: Conceptualization, Funding acquisition, Methodology, Resources, Supervision, Writing – review & editing.
Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This research was carried out under project number T16010c in the framework of the Research Program of the Materials innovation institute (M2i) (www.m2i.nl) supported by the Dutch government and, within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014–2018 and 2019–2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission. The authors would like to thank Research Instruments (RI) GmbH in Germany for supplying the high heat flux exposed monoblock samples.

Appendix A. Hardness measurement

Fig. 11 shows the hardness mapping performed along the armour region of the monoblock following a cyclic heat exposure using the Vickers microindentation technique. A substantial drop in hardness, characteristic of recrystallization can be observed for the regions close to the surface. In contrast, relatively high hardness values occur in the bulk due to the deformed microstructural state. Also, the transition between the recrystallized and the initial microstructure is rather sharp (low vs. high hardness values), with regions close to the cooling tube exhibiting a transition to higher hardness at lower depths than regions located far away from the cooling tube.

Appendix B. Temperature dependent material properties

Fig. 12 depicts the temperature dependent material properties of thermal conductivity (\(\kappa\)), product of mass density and specific heat capacity (\(c\rho\)) used as input for the transient heat analysis.

Fig. 11. The two-dimensional hardness map of the WD-HD plane of the heat exposed monoblock illustrating the recrystallization assisted drop in hardness. The recrystallized regime determined by the hardness measurements coincides with the optical micrograph observations (Fig. 1), with regions close to cooling tube showing a transition to higher hardness at smaller depths, compared to regions at the edge of the monoblock.

Fig. 12. Temperature dependent material properties (a) product of mass density (\(\rho\)) and specific heat capacity (\(c\)), and (b) thermal conductivity (\(\kappa\)) for W, Cu and CuCrZr alloy, used as input in the thermal FEM analyses [50].
Appendix C. Activation energy dependent recrystallized depth

Fig. 13 shows the simulated fully recrystallized depth along the centre and edge of the monoblock following 300 cycles of 10 s exposure as a function of the activation energy. As the activation energy increases, the recrystallization depth decreases with a negligible recrystallization for the highest activation energy, i.e. 550 kJmol⁻¹.

Fig. 13. The activation energy dependent fully recrystallized depth along the centre and edge of the monoblock following 300 cycles of 10 s exposure for 20 MWm⁻².

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