

A PHYSICS-BASED DESCRIPTION OF INTER-GRANULAR HELIUM BEHAVIOUR IN SCIANTIX FOR APPLICATION IN FUEL PERFORMANCE CODES

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ABSTRACT

In this work, we propose a new mechanistic model for the treatment of helium behaviour at grain boundaries in oxide nuclear fuel. The model pairs rate-theory description of helium intra-granular behaviour (diffusion towards grain boundaries, trapping in spherical bubbles, thermal re-solution), developed in a first step, with rate-theory description of helium inter-granular behaviour (diffusion towards grain edges, trapping in lenticular bubbles, thermal re-solution). The proposed model has been implemented in SCIANTIX (meso-scale software designed for coupling with fuel performance codes) and validated against thermal desorption experiments performed on doped UO_2 samples annealed at different temperatures. The overall agreement of the new model with the experimental data is satisfactory, both in terms of integral helium release and of helium release rate, showing an improvement compared to previous mechanistic models, which do not consider the behaviour of helium at grain boundaries. By considering the contribution of helium at grain boundaries it is possible to represent the kinetics of helium release rate at high temperature. Given the uncertainties involved in the initial conditions for the inter-granular part of the model (initial helium concentrations in inter-granular bubbles, and in solution at grain boundaries) and the uncertainties associated to some model parameters for which limited lower-length scale information is available (helium diffusivity at the grain boundaries in particular) the results are complemented by a dedicated sensitivity analysis. This analysis demonstrates that the initial conditions, if chosen in a reasonable range, have limited impact on the results, and confirms that it is possible to achieve satisfying validation results using sound values for the uncertain physical parameters.

1. Introduction

The description of helium behaviour in nuclear fuel is of engineering interest, both in irradiation conditions, since, together with xenon and krypton, it concurs to the gaseous swelling of the fuel pin and gas release in the free volume of the fuel rod, and in storage (since it is produced in large amount due to the α -decay of actinides). Currently, in the state-of-the-art models [1]–[6] used in thermo-mechanical fuel performance codes [7]–[9], the description of gas and helium behaviour is approached in three sequential steps [10], [11]: first production, then intra-granular evolution [12]–[15] and lastly inter-granular evolution [16]. The rate-theory model proposed in this work is similarly designed and is intended for application in fuel performance codes, extending the capabilities of currently available models [10]. The focus is on including the physical description of inter-granular helium behaviour to improve the predicting

48 capabilities of helium evolution in annealing conditions i.e., to be able to reproduce both the
 49 peaks (also that at lower temperature, besides the higher temperature one) of the helium
 50 release rate (see [10] for the results from the intra-granular helium model alone). The model
 51 has been implemented in SCIANTIX [17] (meso-scale software designed for coupling with fuel
 52 performance codes). Given the uncertainties involved in the initial conditions for the inter-
 53 granular part of the model (i.e., the initial helium concentration in inter-granular bubbles, and
 54 in solution at grain boundaries) and the uncertainties associated to some model parameters
 55 for which limited lower-length scale information is available (helium diffusivity at the grain
 56 boundaries in particular) the results are complemented by a dedicated sensitivity analysis. The
 57 description of the model is performed in Section 2, including an introduction to the various
 58 parameter involved (Table 1). The results obtained are showcased and described in Section
 59 3, while the outcomes of the sensitivity analyses on initial conditions and physical model
 60 parameters are reported in Section 4.

61 2. Model Description

62 We herein outline the equations governing the evolution of the in-bubble and single-atom
 63 helium concentrations at grain boundaries

$$\frac{\partial c_{gb}}{\partial t} = S(1 - F) + D_{gb}\nabla^2 c_{gb} - g_{gb}(c_{gb} - c_{s,gb}) + b_{gb}m_{gb} - \nu_{gb}n_{gb} \quad (1)$$

$$\frac{\partial m_{gb}}{\partial t} = SF + g_{gb}(c_{gb} - c_{s,gb}) - b_{gb}m_{gb} + \nu_{gb}n_{gb}$$

64 where S (at $\text{m}^{-2} \text{s}^{-1}$) represents the helium source coming from within the grain, D_{gb} ($\text{m}^2 \text{s}^{-1}$) is
 65 the inter-granular helium diffusion coefficient, c_{gb} (at m^{-2}) is the inter-granular single atom
 66 helium concentration, $c_{s,gb}$ (at m^{-2}) is the solubility of helium at grain boundaries, g_{gb} (s^{-1}) is
 67 the trapping rate, b_{gb} (s^{-1}) is the irradiation induced re-resolution term, m_{gb} (at m^{-2}) is the helium
 68 concentration in inter-granular bubbles, ν_{gb} (bub s^{-1}) is the nucleation term, n_{gb} (at bub^{-1}) is
 69 the number of helium atoms per inter-granular bubble and F (l) is the fractional coverage of
 70 grain faces, which acts as a parameter that distributes (distribution factor) helium reaching the
 71 boundary between inter-granular bubbles and solution.

72 Some considerations are made to develop Eq. 1. We assumed that at the boundary helium
 73 moves on a 2D space, thus diffusion will act accordingly. The spherical Laplacian becomes
 74 cylindrical with the only relevant portion of it being the radial one:

$$D_{gb}\nabla^2 c_{gb} = D_{gb} \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} c_{gb} \quad (2)$$

75 As far as the source term is concerned, we said that the source of grain boundary helium
 76 comes from within the grain itself. Diffusion of intra-granular helium towards the boundary is
 77 what represents our inter-granular source. This makes the grain boundary evolution dependent
 78 on the intra-granular behaviour.

79 For S to be expressed coherently, the intra-granular helium single atom concentration c_{ig}
 80 (at m^{-3}) needs to be rescaled on a 2D space by means of the surface to volume ratio of the
 81 spherical grain radius which is equal to one third of the spherical grain radius itself, i.e., $c_{ig,gb} =$
 82 $\frac{a}{3} c_{ig}$, where $c_{ig,gb}$ (at m^{-2}) is the contribution to grain boundary helium coming from within the
 83 grain and a (m) is the spherical grain. Thus, the expression of S (which corresponds to the
 84 intra-granular concentration diffusing out of the spherical grain and entering a cylindrical grain
 85 face, coupling intra- and inter-granular behaviour) becomes:

$$S = -\frac{a}{3} D_{ig} \frac{1}{r_*^2} \frac{\partial}{\partial r_*} r_*^2 \frac{\partial}{\partial r_*} c_{ig} \quad (3)$$

86 where D_{ig} is the intra-granular diffusion coefficient ($\text{m}^2 \text{s}^{-1}$). The Laplacian of the source
 87 remains expressed in spherical coordinates because the diffusion which produces S takes
 88 place in the intra-granular framework.

89 In analogy with the intra-granular model [10], we included the helium solubility at grain
 90 boundaries that follows Henry's law, $c_{s,gb} = \frac{a}{3} k_H p_{gb}$, where k_H is the Henry constant [18], p_{gb}
 91 is the helium pressure at grain boundaries and $\frac{a}{3}$ is the surface to volume ratio (used as
 92 conversion factor). The solubility leads to a thermally activated re-resolution of helium single
 93 atoms from bubbles in the form:

$$\gamma_{gb} m_{gb} = g_{gb} c_{s,gb} \quad (4)$$

94 where γ_{gb} (s^{-1}) is the inter-granular thermal re-resolution rate.

95 In annealing conditions, the irradiation induced re-resolution rate is null, $b_{gb} = 0$, and it is
 96 assumed that a bubble population is formed at the first time-step and then it evolves along the
 97 experiment [10], [19]; thus, if we substitute Eqs. 2, 3 and 4 into Eq. 1, the inter-granular
 98 equations become:

$$\frac{\partial c_{gb}}{\partial t} = -\frac{a}{3} D_{ig} \frac{1}{r_*^2} \frac{\partial}{\partial r_*} r_*^2 \frac{\partial}{\partial r} c_{ig} (1 - F) + D_{gb} \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} c_{gb} - g_{gb} c_{gb} + \gamma_{gb} m_{gb} \quad (5)$$

$$\frac{\partial m_{gb}}{\partial t} = -\frac{a}{3} D_{ig} \frac{1}{r_*^2} \frac{\partial}{\partial r_*} r_*^2 \frac{\partial}{\partial r} c_{ig} F + g_{gb} c_{gb} - \gamma_{gb} m_{gb}$$

99 These equations are then coupled with those defining the model for the intra-granular helium
 100 evolution [10]. The various parameters involved in the inter-granular model can be found in
 101 **Table 1**.

102

| Symbol | Description | Formula | units | Reference |
|----------------|---------------------------------------|--|------------------------------------|-------------------|
| D_{ig} | Intra-granular diffusion coefficient | $2.0 \cdot 10^{-10} \exp(-2.12/kT)$ | $\text{m}^2 \text{s}^{-1}$ | [10],[20] |
| D_{gb} | Inter-granular diffusion coefficient | $10^3 \cdot D_{ig}$ | $\text{m}^2 \text{s}^{-1}$ | Present work |
| g_{gb} | Inter-granular trapping rate | $2\pi D_{gb} N_{gb} / \ln(1/R_{gb} \sqrt{\pi N_{gb}})$ | s^{-1} | Present work,[21] |
| $c_{s,gb}$ | Inter-granular helium solubility | $\frac{a}{3} k_H p_{gb}$ | at m^{-2} | [10], [22 – 24] |
| k_H | Henry's constant | $4.1 \cdot 10^{24} \exp(-0.65/kT)$ | $\text{at m}^{-3} \text{MPa}^{-1}$ | [10], [18] |
| γ_{gb} | Inter-granular thermal re-resolution | $\frac{2\pi D_{gb}}{\ln\left(\frac{1}{R_{gb} \sqrt{\pi N_{gb}}}\right)} \frac{a}{3} k_H \frac{kT}{V_{gb}} Z$ | s^{-1} | Present work |
| p_{gb} | Inter-granular helium bubble pressure | $kTZ n_{gb} / V_{gb}$ | Pa | |
| F | Fractional coverage | $N_{gb} A_{gf}$ | / | [16] |
| V_{gb} | Average inter-granular bubble volume | $4\phi(\theta) \pi R_{gb}^3 / (3 \sin^3(\theta))$ | m^3 | [16] |
| $\phi(\theta)$ | Semi-dihedral factor of a bubble | $1 - 1.5 \cos(\theta) + 0.5 \cos^3(\theta)$ | / | [16],[25] |

103 **Table 1:** Parameters involved in the inter-granular model proposed in this work.

104

105 **3. Results**

106 For validation purposes, we tested the predictive capabilities of the model against a set of data
107 on helium release and release rate collected by Talip et al. [19] during annealing
108 measurements. The experiment was performed on UO₂ samples doped with 0.1 wt.% of
109 additive containing 66.7 wt.% of ²³⁸PuO₂, whose α-decay produced helium atoms within the
110 sample during an aging period of 15 years in a glovebox with inert atmosphere (N₂). The
111 samples were then annealed in a Knudsen Effusion Mass Spectrometer and helium release
112 was measured using a Quantitative Gas Measurement System (Q-GAMES) [26]. For the sake
113 of brevity we decided to present only the results obtained for one of the temperature histories
114 available [19]. In particular, the profile considered in this work is shown in **Figure 1**. We focused
115 on the 1800 K irradiation history to show the improvement in predicting the double helium
116 release peak brought about by the coupled intra- and inter-granular description with respect to
117 the result from the intra-granular model alone, reported in [10].

118 The temperature history is characterised by a heat up ramp of 30 minutes at 10-20 K min⁻¹
119 with a subsequent hold of the temperature, at a value of 1800 K, for 1-3 h. After the plateau,
120 the temperature is decreased to 800 K.

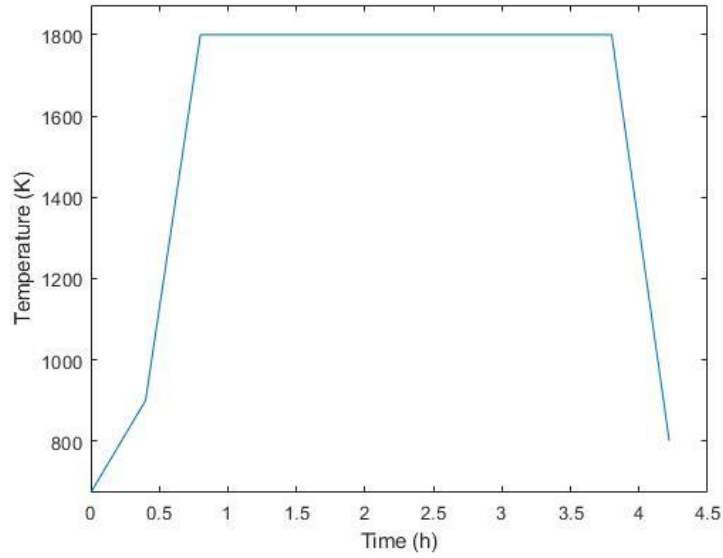
121 We choose to present the results obtained at 1800 K because, in this annealing history, the
122 improvement provided by the novel inter-granular model in predicting the helium release
123 behaviour is mostly appreciable.

124 For the history considered, the behaviour of helium fractional release and helium release rate
125 is reported. The results of the model incorporating the contribution of the grain boundaries are
126 also compared to the previous version of the model (only intra-granular contribution) and with
127 the aforementioned experimental results [19]. Modelling assumptions, necessary for the set-
128 up of the SCIANTIX simulation are made on the inter-granular helium diffusion coefficient and
129 on the fraction of helium initially considered at grain boundaries. In particular a reference value
130 of 10% of the helium produced is taken for the fraction of helium initially present at boundary
131 and the ratio D_{gb}/D_{ig} is assumed to be 10³ [27].

132 **Figure 2** shows that the inclusion of a model treating helium behaviour at grain boundaries
133 provides a further step to enlighten the physical behaviour of this gas inside nuclear fuel. The
134 helium release at 1800 K is improved but still slightly underestimated. This could be due to the
135 uncertainty on the initial values of helium at the boundary (as explained in the following
136 section). Also, the residual underestimation during the annealing at constant temperature calls
137 for further extensions of the intra-granular helium model capabilities, controlling the release at
138 this stage. As far as the helium release rate is concerned, the most noticeable remark is the
139 double peak in the release rate of the 1800 K profile, as shown by the measured profile [19].
140 The presence of a peak at lower temperature, followed by a second one at higher temperature,
141 is coherent with the fact that, as stated by Martin et al. [28], [29], the release of helium occurs
142 in two successive stages. The first stage corresponds to the release of helium which is located
143 a few microns either side of grain boundaries, where faster helium diffusion occurs (i.e., regions
144 with higher diffusion rate). This is also consistent with the slightly lower activation energy for
145 grain boundary diffusion obtained by Garcia et al. [27] and shown in **Figure 4** below, although
146 the uncertainty on the activation energy is large. The second stage of helium release should
147 occur via the slow re-resolution and release of gas atoms trapped within grains.

148 Thus, helium at grain boundaries plays a relevant role on the overall helium behaviour and the
149 evidence that the proposed model can correctly predict the two stages in which release occurs,
150 is a promising achievement.

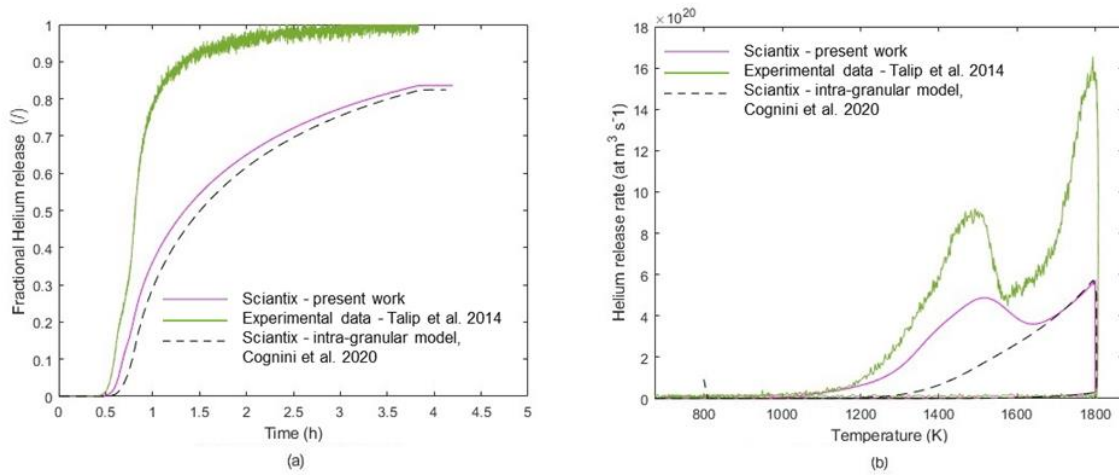
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153 **Figure 1:** Temperature history of the annealing experiment [19] at 1800 K herein considered.

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155

156 **Figure 2:** Comparison of SCIANTIX fractional helium release (a) and helium release rate (b)
 157 with experimental data provided by Talip et al.[19] from the temperature history at 1800K. The
 158 black dashed line represents the results from Cognini et al.[10] and the purple line the present
 159 development including grain boundary treatment.

160 4. Sensitivity analyses: parametric studies

161 Given the lack of experimental information on helium at grain boundaries, some assumptions
162 were made on the initial values of some parameters of the model, namely the initial fraction of
163 helium stored at the grain boundaries at the beginning of the annealing test and its distribution
164 among inter-granular bubbles and inter-granular solution, together with the diffusivity of helium
165 at the grain boundaries.

166 The hypothesis of considering an initial portion of the helium produced in the samples at grain
167 boundaries comes from Martin et al. [28], who stated that a fraction of the helium initially
168 produced in a sample is close enough to the boundaries to be considered at grain boundaries.
169 As for the exact value for this initial boundary contribution, no experimental data are available.
170 To throw light into this fundamental model parameter, mandatory for the initialization of the
171 SCIANTIX simulation, a sensitivity analysis was performed, and a 10% fraction of the helium
172 produced emerged as a value showing promising results (as can be seen from **Figure 2**). This
173 value was then compared to others within an uncertainty range. The two extreme values of the
174 interval chosen are 0%, that comes from the original model by Cognini et al. [10] which neglects
175 the treatment of helium at grain boundary, and 20%, which emerged during the sensitivity
176 analysis as the value beyond which the model started overestimating all the release rate peaks
177 attributable to the helium at boundaries contribution. It is possible to see from **Figure 3(a)** that,
178 within the chosen range of uncertainty, the effect on the overall release is a variation of around
179 3.5%, or a $\pm 1.75\%$ with respect to the reference value (10%) of helium initially assumed to be
180 at boundary.

181 Concerning how helium at grain boundaries is initially split between inter-granular solution and
182 inter-granular bubbles, it is relevant to see how this subdivision could impact the fractional
183 release and the release rate. To understand the influence of the aforementioned division, once
184 again the behaviour determined by the annealing history at 1800 K is considered. Since no
185 assessed data are available, this case also required a proper sensitivity analysis. The fraction
186 of helium in bubbles was made to vary in a range between 0% to 50% of the total helium initially
187 present at grain boundaries. **Figure 3(c)** and **Figure 3(d)** show that the initial helium
188 distribution bears little to no effect on the overall fractional release, but it induces some
189 changes on the first peak in helium release rate. This is reasonably within expectations, since
190 how helium is distributed between bubbles and solution does not affect how much helium will
191 ultimately be released (the integral of the release is not affected), while, on the other hand,
192 having more helium in bubbles at the initial stages of release means that more gas needs to
193 return in solution before release, slightly reducing the rate and vice versa (The derivative of
194 the release is what perceives the effect of the split). This effect is then reflected on the first
195 peak because it is the one associated to the release of helium initially present at grain
196 boundaries (as already stated in Section 3). Nevertheless, we can see that even along a 50%
197 range of uncertainty the effect of this parameter is relatively small. Future data collection on
198 this open issue could provide a more detailed insight on how this initial split should be treated.

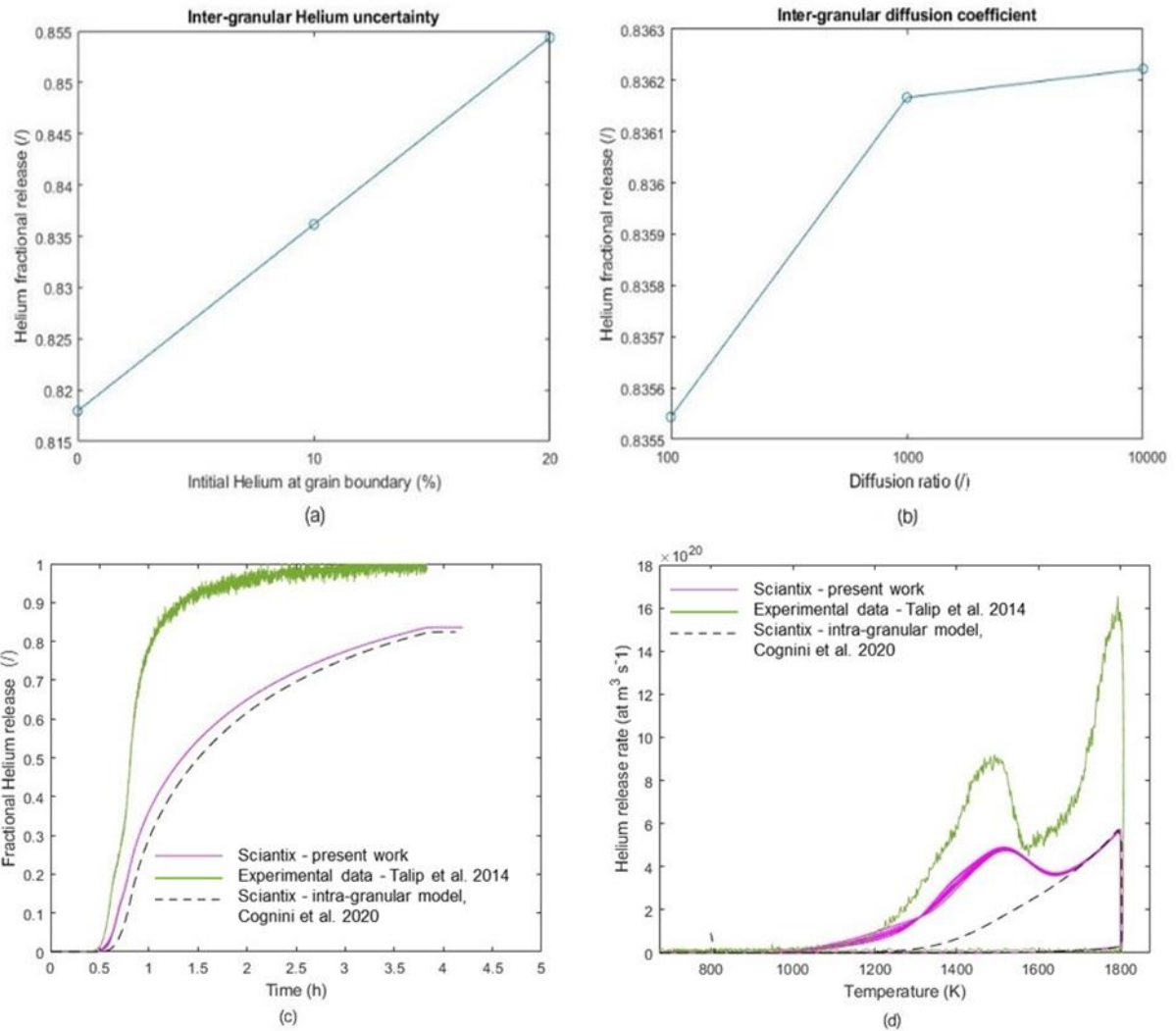
199 As far as the diffusion coefficient is concerned, the lack of experimental data for this specific
200 case and, in general, for the definition of a specific coefficient, led to the choice of considering
201 the same diffusion correlation adopted by Cognini et al. [10] in the intra-granular only version
202 of this model, but increased by a certain factor defined by the ratio D_{gb}/D_{ig} (hence, keeping
203 the same slope of the correlation in [10], coming from [20]).

204 Interesting results obtained by Garcia et al. [27] are presented in **Figure 4**, that shows values
205 at different temperatures of the helium intra-granular and inter-granular diffusion coefficients
206 in UO_2 polycrystalline samples. The experimental scatter and the scarcity of data provide a
207 justification for considering that the activation energy for bulk and grain boundary diffusion are
208 similar in this work. The experimental scatter and the scarcity of data provide a justification for

209 considering that the activation energy for bulk and grain boundary diffusion are similar in this
210 work. From those results it is thus possible to evaluate the diffusion ratio. Comparing the intra-
211 granular and inter-granular experimental data reported in **Figure 4** it is possible to determine
212 that the diffusion ratio varies in a range between $D_{gb}/D_{ig} \sim 10^2$ and $D_{gb}/D_{ig} \sim 10^4$. At the
213 highest temperature at which data were collected (1373 K), the value of the ratio is
214 $D_{gb}/D_{ig} \sim 10^3$. Since this last value of the ratio is achieved at a temperature that is the closest
215 (among the ones in **Figure 4**) to the holding temperature of the annealing history considered,
216 it is assumed as the reference value for the diffusion ratio adopted in this work.

217 We can see from **Figure 3(b)** that the impact of the diffusion coefficient uncertainty on the
218 fractional helium release is basically negligible for the temperature profile considered (and also
219 for the other cases analysed in [10]). The impact of the diffusion coefficient is more significant
220 on the helium release rate, since a smaller diffusion coefficient implies a first peak significantly
221 delayed while a greater diffusion coefficient implies a first release rate peak occurring at lower
222 temperature values.

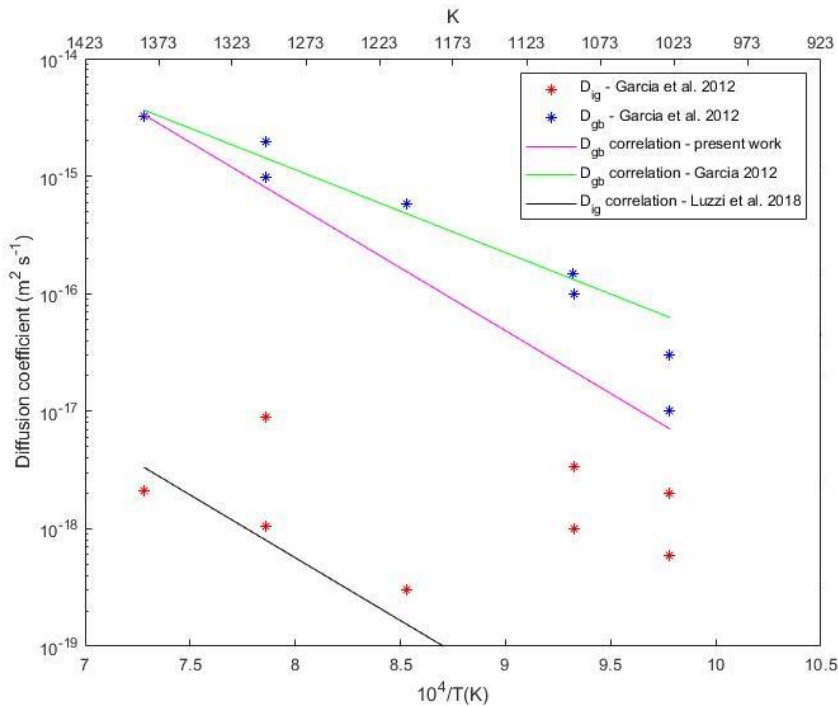
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225 **Figure 3:** Effects of the uncertainty analysis on helium release behaviour: (a) effect of the
 226 fraction of helium initially present at grain boundaries on the fractional release, (b) effect of the
 227 diffusion coefficient on the fractional release, (c) bundle of curves that shows the effects on
 228 fractional release of how the fraction of helium initially present at grain boundaries is split
 229 between bubbles (in a range between 0% and 50%) and solution, (d) bundle of curves that
 230 shows the effects on release rate of how the fraction of helium initially present at grain
 231 boundaries is split between bubbles (in a range between 0% and 50%) and solution. The
 232 curves calculated with the reference model parameters are already reported in Figure 2 and
 233 correspond to the centre of the bundles in both plots (c) and (d).

234



235

236 **Figure 4:** Helium diffusion coefficients within the grain (red data) and around the grain
 237 boundaries (blue data) [27]. Different correlation are reported on the graph: the correlation
 238 proposed for grain boundary diffusion in the samples studied by Garcia et al. (green line), the
 239 correlation adopted for grain boundary helium in this work (purple line) and the correlation
 240 adopted in the intra-granular helium model [10], [20].

241

242 5. Conclusion

243 In this work a new model for the description of helium evolution at grain boundaries is
 244 proposed. The model is implemented in SCIANTIX and aims at improving the predictive
 245 capabilities on helium behaviour by including a description of helium evolution at grain
 246 boundaries. The model is validated against a set of data collected during annealing
 247 experiments on UO_2 performed by Talip et al. (2014). The results show that the inclusion of a
 248 model treating helium behaviour at grain boundaries provides a promising overall improvement
 249 with respect to the version where the inter-granular contribution to helium evolution was not
 250 considered. This improvement can especially be appreciated on the release rate of the 1800
 251 K history where the experimentally observed double peak, previously absent in the state-of-
 252 the-art predictions, becomes visible. The parametric analysis on some critical parameters
 253 showed that, within a reasonable range, they bear little impact on the final value of the release.
 254 Some of the features of the models can still be improved. First of all, a better description of the
 255 distribution factor and further investigation could identify the best approach to define this
 256 parameter. Then a more detailed experimental knowledge would allow to improve the quality
 257 of the assumptions made for the input parameters. Additional analyses could involve the
 258 identification of the “optimal” model parameters (in terms of initial fraction of helium at the grain
 259 boundary and inter-granular diffusion coefficient) providing the best agreement with the
 260 available experimental data on helium release and release rate. Lastly the definition of a
 261 proper diffusion coefficient rather than a simple diffusion ratio would allow accounting for a
 262 more precise evaluation of the diffusion at grain boundaries.

263

264 **Acknowledgements**

265 This work has received funding from the Euratom research and training programme 2019-
266 2020 under grant agreement No 945077 (PATRICIA project).

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