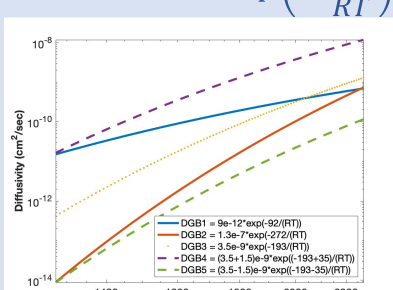
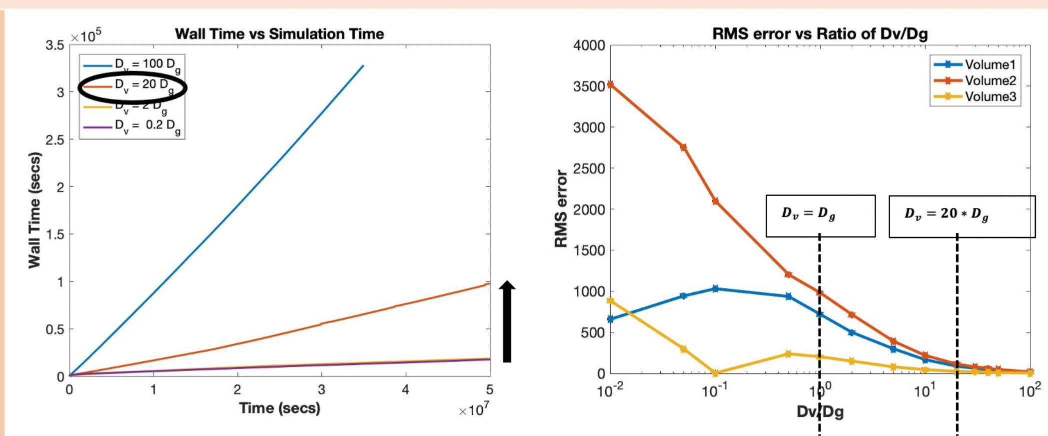
	Name of the material property	Value	Paper Title
1	Atomic volume of U atom in $\mathbf{UO_2}$ crystal	$0.0409\ nm^3$	Phase-field modeling of fission gas bubble growth on grain boundaries and triple junctions in UO_2 nuclear fuel, Larry et al. (2019), JNM V-161, 35-45
2	$\mathbf{C_{g,bubble,equilibrium}}$	0.454	"
3	$\mathbf{C_{v,bubble,equilibrium}}$	0.546	"
4	Fission Yield of Xe	$Y_{Xe} = 0.2156$	IAEA Handbook of Nuclear Data for Safeguards, International Atomic Energy Agency. Chain fission yields. https://www-nds.iaea.org/sgnucdat/c1.htm; accessed 13-Apr-2017.
5	Fission Rate Density	$\dot{F} = 1.09 * 10^{13}\ \frac{fission}{cm^3 - sec}$	Fundamental Aspects of Nuclear Reactor Fuel Elements, D.R. Olander (1976)
6	GB Energy	$1.56 - 5.87 * 10^{-4}T \pm 0.3\frac{\mathrm{J}}{\mathrm{m}^2}$	Mechanistic grain growth model for fresh and irradiated UO_2 nuclear fuel, Tonks et al., JNM V-543, 152576 [2021]
7	Surface Energy	2* GB Energy	Surface, grain boundary and interfacial energies in UO_2 and UO_2-Ni, Nikolopuolos [1977] Surface energy measurements on UO2 – a critical review, Hall et al., JNM, 148 (1987), pp. 237-256
8	Vacancy and Interstitials Migration Energy	$\Delta H_{Vo}^m = 0.5\ to\ 0.6\ ev$ $\Delta H_{Oi}^m = 0.8\ to\ 1\ ev$ $\Delta H_{Vu}^m = 2.4\ ev$ $\Delta H_{Ui}^m = 2.0\ ev$	Atomic Transport Properties in U02 and Mixed Oxides (U,Pu) O2, Matzke: J. Chem. SOC., Faraday Trans. 2, 1987,83, 1121-1142
9	Vacancy and Interstitials Diffusivity	$D_{U\,vac} = 2 * 10^{-3}(\frac{cm^2}{s})$ $\exp\left(-\frac{2.4}{KT}\right)$ $D_{U\,Int} = 1 * 10^{-1}(\frac{cm^2}{s})$ $\exp\left(-\frac{2.0}{KT}\right)$	Atomic Transport Properties in U02 and Mixed Oxides (U,Pu) O2, Matzke: J. Chem. SOC., Faraday Trans. 2, 1987,83, 1121-1142
10	Vacancy Formation Energy	3 eV	The diffusion coefficients of gaseous and volatile species during the irradiation of uranium dioxide, Turnbull et. al., JNM, 107 (168-184), [1982]
11	Gas Formation Energy	3 eV	Phase-field simulations of intragranular fission gas bubble evolution in UO_2 under post-irradiation thermal annealing, Yulan Li [2013] Phase-field modeling of fission gas bubble growth on grain boundaries and triple junctions in UO_2 nuclear fuel, Larry Aagesen [2019]

12	Gas bulk diffusivity	$0.0212\frac{nm^2}{s}\ (T = 1200k)$	The diffusion coefficients of gaseous and volatile species during the irradiation of uranium dioxide, Turnbull et. al., JNM, 107 (168-184), [1982]
13	$\boldsymbol{K_v^{matrix} = K_g^{matrix}}$ (Curvatures of the parabolas)	$7.07 * 10^9 \frac{J}{m^3}$ $(Actual: 4.81 * 10^{11} \frac{J}{m^3})$	Phase-field simulations of intragranular fission gas bubble evolution in UO_2 under post-irradiation thermal annealing, Yulan Li [2013]
14	$\boldsymbol{K_v^{bubble} = K_g^{bubble}}$ (Curvatures of the parabolas)	$9 * 10^{10} \frac{J}{m^3}$	Phase-field simulations of intragranular fission gas bubble evolution in UO_2 under post-irradiation thermal annealing, Yulan Li [2013]
15	GB Mobility	$M_o \exp\left(-\frac{Q}{RT}\right)$	Mechanistic grain growth model for fresh and irradiated UO_2 nuclear fuel, Tonks et al., JNM V-543, 152576 [2021]
16	Mobility Prefactor	$M_o = 2.14 \pm 0.15\ * 10^{-7}$	Mechanistic grain growth model for fresh and irradiated UO_2 nuclear fuel, Tonks et al., JNM V-543, 152576 [2021]
17	Activation Energy	$290 \pm 22 \frac{Kj}{mol}$	Mechanistic grain growth model for fresh and irradiated UO_2 nuclear fuel, Tonks et al., JNM V-543, 152576 [2021]
18	Kappa, $\boldsymbol{\kappa}$	$\frac{3}{4} * GB_{energy} * GB_{width}$	Quantitative analysis of grain boundary properties in a generalized phase field model for grain growth in anisotropic systems, Moelans, Physical Review B 78, 024113 [2008]
19	$\boldsymbol{m\ (Mu)}$	$6 * \frac{GB_{energy}}{GB_{Width}}$	Quantitative analysis of grain boundary properties in a generalized phase field model for grain growth in anisotropic systems, Moelans, Physical Review B 78, 024113 [2008]
20	$\boldsymbol{L}$	$\frac{4}{3} * \frac{GB_{mobility}}{GB_{width}}$	Quantitative analysis of grain boundary properties in a generalized phase field model for grain growth in anisotropic systems, Moelans, Physical Review B 78, 024113 [2008]
21	GB Diffusivity	$D_{GB,Upper} = 9 * 10^{-12} * \exp\left(-\frac{92}{RT}\right)$ $D_{GB,Lower} = 1.3 * 10^{-7} * \exp\left(-\frac{272}{RT}\right)$ 	On the role of grain boundary diffusion in fission gas release, D. Olander (2001), JNM, V-288, P: 137-147
22	GB Thickness	0.5 nm	Grain growth and pore coarsening in dense nano-crystalline UO2+x fuel pellets, T. Yao, 2017

Name of the property	Calculation
Corresponding chemical potential value for the gas concentration = 0 on the left boundary	$\mu_{gas} = V_a * \frac{\partial f_{chem_{matrix}}}{\partial c_{gas}} = V_a * k_{gas}^{matrix} * (C_{gas} - C_{gas,equilibrium})$ $= 0.0409\, nm^3 * 3.00625e3 \left(\frac{ev}{nm^3}\right) * (0 - 2.512 * 10^{-13}) = -3.1 * 10^{-11}\, eV$
GB Diffusivity	$D_{GB,Upper} = 9 * 10^{-12} * \exp\left(-\frac{92}{RT}\right)$ $D_{GB,Lower} = 1.3 * 10^{-7} * \exp\left(-\frac{272}{RT}\right)$ $D_{GB,mean.} = 3.5 \pm 1.5 * 10^{-9} * \exp\left(-\frac{193 \pm 35}{RT}\right)$
GB Diffusivity Modeling	$D_{GB,\,modeling} = \frac{GB_{thickness,\ actual} * D_{GB,\,actual} (= D_{GB,mean})}{GB_{thickness,modeling} * Fraction\ of\ area\ under\ the\ curve}$ $= \frac{0.5\, nm * D_{GB,actual}}{30nm\ * 0.2}$ $= \frac{1}{12} * D_{GB,\,actual}\ for\ GB_{width} = 30nm$
Fraction of area under the curve	$\eta_1 = \frac{1}{2} * (1 - \tanh(\frac{x}{0.3}))$ $\eta_2 = 1 - \eta_1 = \frac{1}{2} * (1 + \tanh(\frac{x}{0.3}))$ Area under the curve: $\int_0^1 16 * \eta_1^2 * (1 - \eta_1)^2\, d\eta_1$ $= \int_0^1 16 * \left[\frac{1}{2} * \left(1 - \tanh\left(\frac{x}{0.3}\right)\right)\right]^2 * \left[\frac{1}{2} * \left(1 + \tanh\left(\frac{x}{0.3}\right)\right)\right]^2 * dx = 0.2$
Vacancy Diffusivity = 20 * Gas Diffusivity	
Bulk Diffusivity of Gas (in $\frac{m^2}{s}$)	$D = D_1 + D_2 + D_3 =$ $7.6 * 10^8 * \exp\left(-\frac{35250}{T}\right) + 1.7835 * 10^7 * \sqrt{\frac{\dot{F}}{Y_{Xe}}} * \exp\left(-\frac{13800}{T}\right) + 2 * 10^5 * \frac{\dot{F}}{Y_{Xe}}$

Diffusivity heterogeneity of gas	$D_{gas} = D_g^{bulk}(1 - h_b - 8\sum_{i=1}^{n}\sum_{j=1,j!=i}^{n}\eta_i^2\eta_j^2) + D_g^{GB}(8\sum_{i=1}^{n}\sum_{j=1,j!=i}^{n}\eta_i^2\eta_j^2) + D_g^{bubble}\boldsymbol{h_b}$
Diffusivity heterogeneity of vacancies	$D_{vacancy} = 20 * [D_v^{bulk}(1 - h_b - 8\sum_{i=1}^{n}\sum_{j=1,j!=i}^{n}\eta_i^2\eta_j^2) + D_v^{GB}\left(8\sum_{i=1}^{n}\sum_{j=1,j!=i}^{n}\eta_i^2\eta_j^2\right) + D_v^{surf}(\boldsymbol{16\eta_b^2(1-\eta_b)^2})]$
Gas Concentration	$c_g = h_b * V_a * \rho_g^{bub} + h_m * v_a * \rho_g^{matrix}$
Vacancy concentration	$c_v = h_b * V_a * \rho_v^{bub} + h_m * v_a * \rho_v^{matrix}$
Density of gas in bubble phase	$\rho_g^{bub} = \frac{\mu_g}{v_a^2 * k_g^{bub}} + \frac{c_{g,bub}^{eq}}{v_a}$
Density of gas in matrix phase	$\rho_g^{matrix} = \frac{\mu_g}{v_a^2 * k_g^{matrix}} + \frac{c_{g,matrix}^{eq}}{v_a}$
Density of vacancy in bubble phase	$\rho_v^{bub} = \frac{\mu_v}{v_a^2 * k_v^{bub}} + \frac{c_{v,bub}^{eq}}{v_a}$
Density of vacancy in matrix phase	$\rho_v^{\boldsymbol{matrix}} = \frac{\mu_v}{v_a^2 * k_v^{matrix}} + \frac{c_{v,matrix}^{eq}}{v_a}$
Gas Mobility	$D_g * \chi_g$
Vacancy Mobility	$D_v * \chi_v$
Gas Susceptibility	$\chi_g = \frac{1}{v_a^2} * \left(\frac{h_m}{k_g^{matrix}} + \frac{h_b}{k_g^{bub}}\right)$
Vacancy Susceptibility	$\chi_v = \frac{1}{v_a^2} * \left(\frac{h_m}{k_v^{matrix}} + \frac{h_b}{k_v^{bub}}\right)$

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