

Integrated computational study of material lifetime in a fusion reactor environment

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Introduction

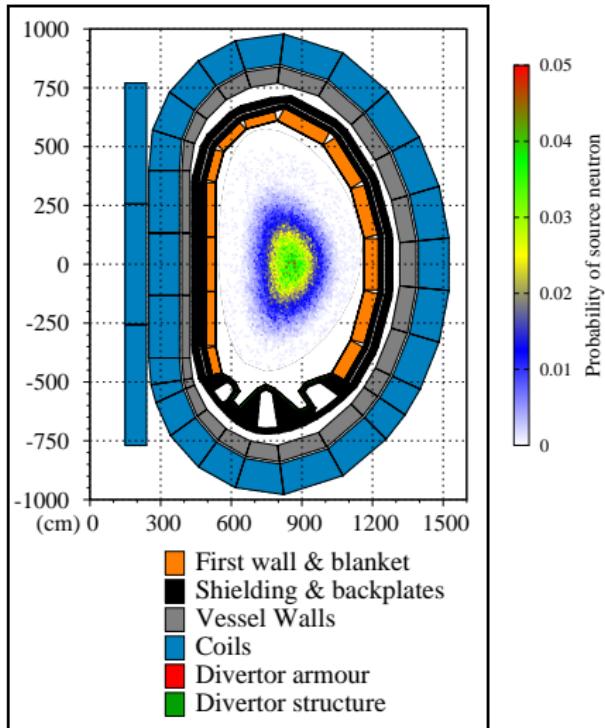
- The neutrons generated in fusion plasmas bombard the surrounding materials...
 - ▶ $\sim 10^{15}$ neutrons $\text{cm}^{-2} \text{ s}^{-1}$ expected on plasma-facing first wall (FW) in DEMO
- ...and induce nuclear reactions
 - ▶ e.g. $^{56}\text{Fe}(n, \gamma)^{57}\text{Fe}$, $^{12}\text{C}(n, \alpha)^9\text{Be}$, $^{64}\text{Cu}(n, p)^{63}\text{Ni}$
- During reactor operation these *transmutations* will produce new elements, including gases (helium and hydrogen)
- Accumulation of these impurities could significantly alter the structural and mechanical properties of materials
 - ▶ Hardening, swelling, gas-induced embrittlement, etc.
- A full picture of the transmutation response and consequences requires:
 - ▶ knowledge of the irradiation conditions
 - ▶ calculation of the burn-up of materials
 - ▶ modelling the effect of impurities

- 1. Neutron transport calculations (neutronics) with MCNP
 - ▶ predicts the irradiation environment for components within a given reactor design
 - ▶ delivers neutron fluxes and energy spectra
- 2. Inventory calculations with FISPACT
 - ▶ neutron spectrum and flux as input
 - ▶ calculates the activation and burn-up (transmutation) of materials
 - ▶ quantifies the changes to material composition in time
- But the absolute transmutation numbers do not inform without models to predict consequences
- 3. Modelling of material properties (atomistic or otherwise)
 - ▶ First attempt:
 - Helium embrittlement of grain boundaries in different materials using production rates from FISPACT

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1. Neutronics: DEMO model for MCNP

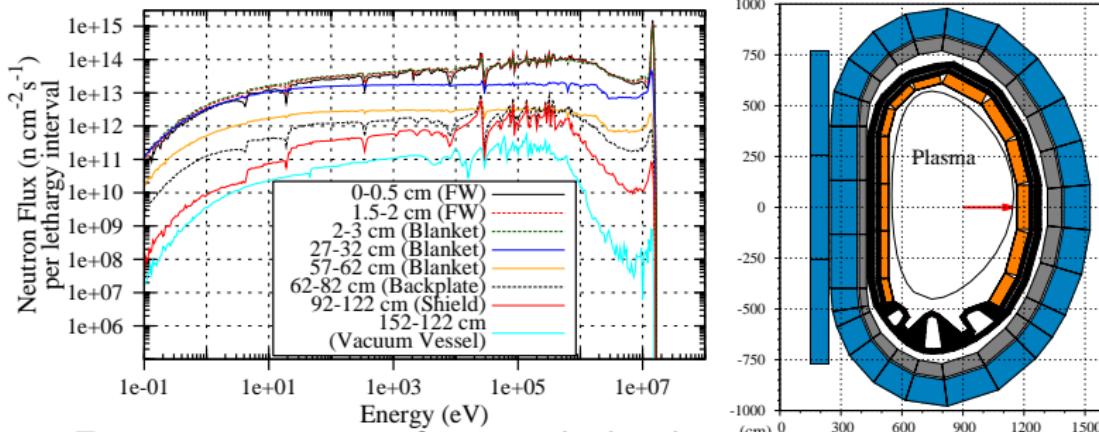
- 2009 model designed using **HERCULES¹**
- 2.7 GW fusion power output
- Cell-based geometry
- Solid Be+Li tritium breeding blanket + W divertor + He cooling
- Neutrons transported through model from a correctly defined fusion-plasma source
- Simulation of sufficient neutrons to provide good statistics



¹Pampin and Karditsas, 2006 *Fusion Eng. Des.*, **81** 1231-7

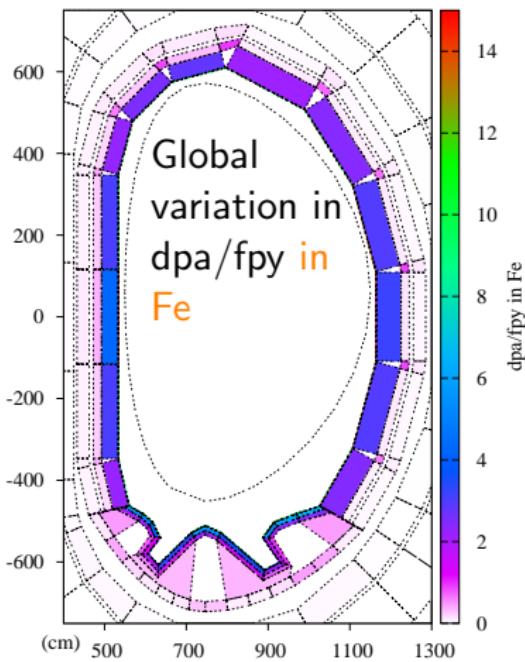
1. Neutronics: example spectra

- Neutron spectra as a function of depth into outboard equatorial First Wall (FW):



- Energy spectrum softens with depth
- Total flux also falls:
 - ▶ Total in 2 cm FW is $8.25 \times 10^{14} \text{ n cm}^{-2} \text{ s}^{-1}$
 - ▶ In final 5 cm of blanket drops to $3.90 \times 10^{13} \text{ n cm}^{-2} \text{ s}^{-1}$
 - ▶ In vessel walls it is only $1.38 \times 10^{12} \text{ n cm}^{-2} \text{ s}^{-1}$
- Variation is complex, so standard practice is to calculate integrated quantity → e.g. dpa

1. Integrated results: dpa



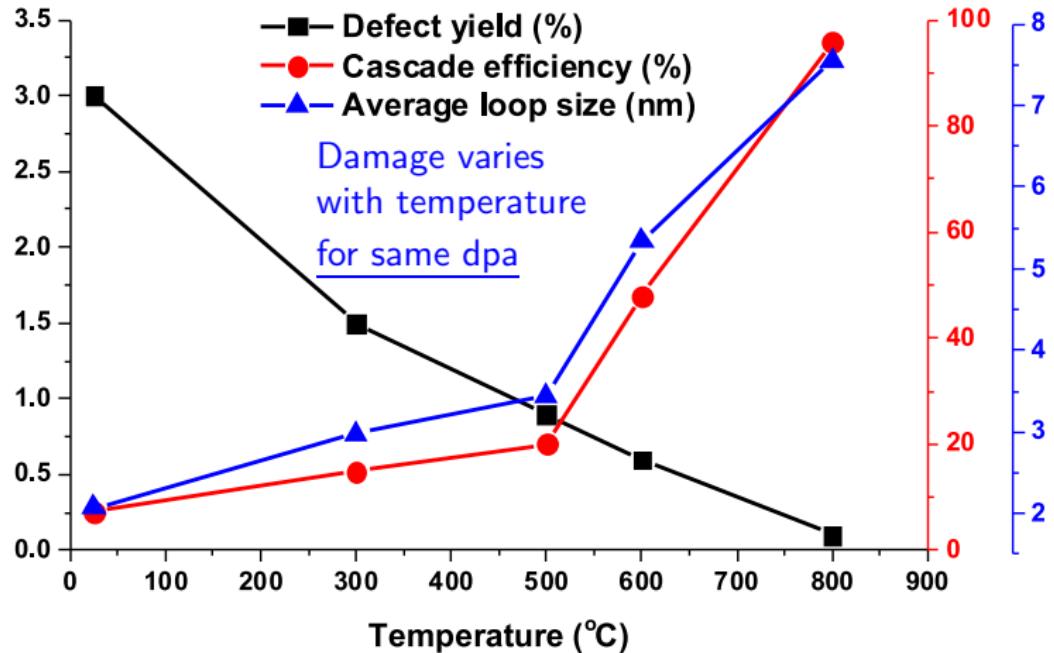
- Displacements per atom (dpa): Integrated measure of total exposure
 - ▶ Spectra and fluxes merged with **Material dependent nuclear data (EFF 1.1)**
- shows the variation in “exposure” with position
- dpa/fpy in Fe in FW armour is ~ 3 times higher than in blanket
- Note: dpa estimates do not take into account the time evolution of radiation damage and give no direct information about changes to microstructure or properties

Caution with dpa interpretation

X. Yi¹, M.L. Jenkins¹, M.A. Kirk², S.G. Roberts¹ – 2012

¹Department of Materials, University of Oxford; ²Argonne National Laboratory

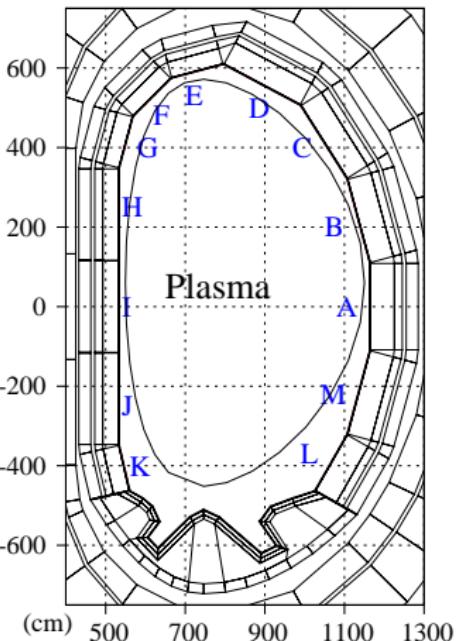
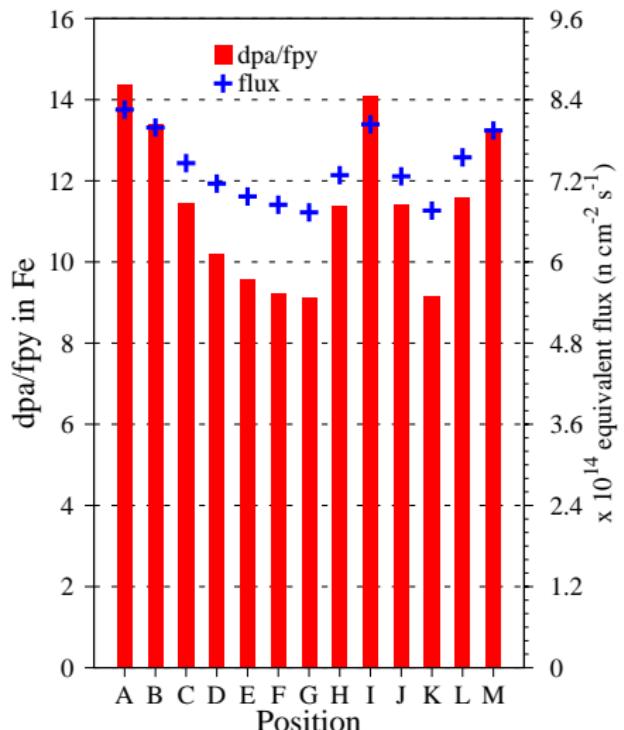
- self-ion irradiation of pure W to 0.01 dpa at a range of temperatures



- However, dpa is a convenient atom-based measure of irradiation exposure

1. dpa: variation with poloidal angle in FW armour

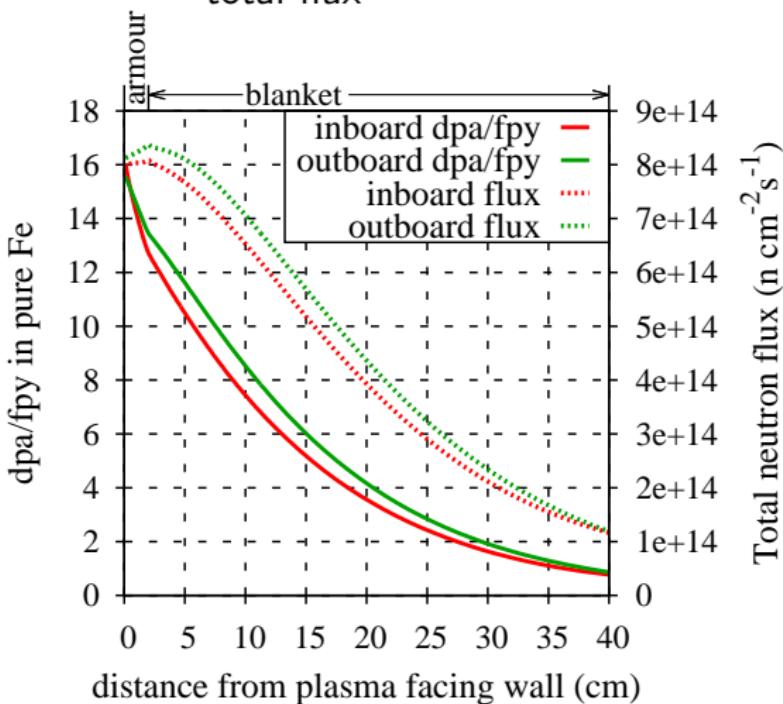
- Exposure measured as dpa/fpy in Fe for the 2 cm FW armour



- poloidal variation in dpa/fpy follows variation in total flux...

1. dpa: variation with depth

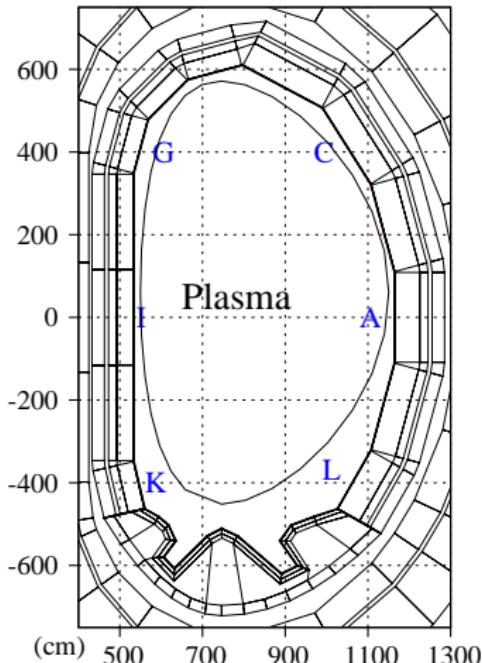
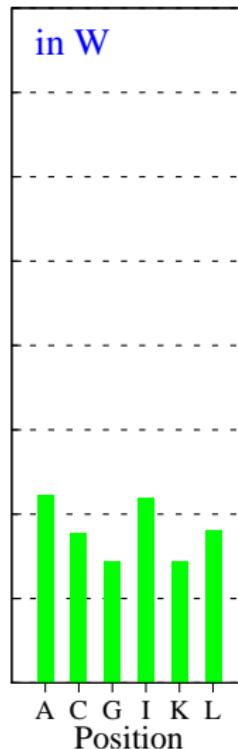
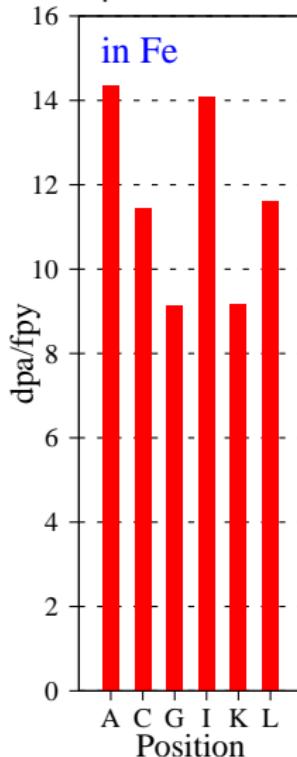
- ... but dpa variation does not always follow change in total flux



- dpa/fpy in Fe and total flux as a function of depth into outboard equatorial FW
- total flux initially increases due to neutron multiplication
- but equivalent dpa/fpy is always decreasing

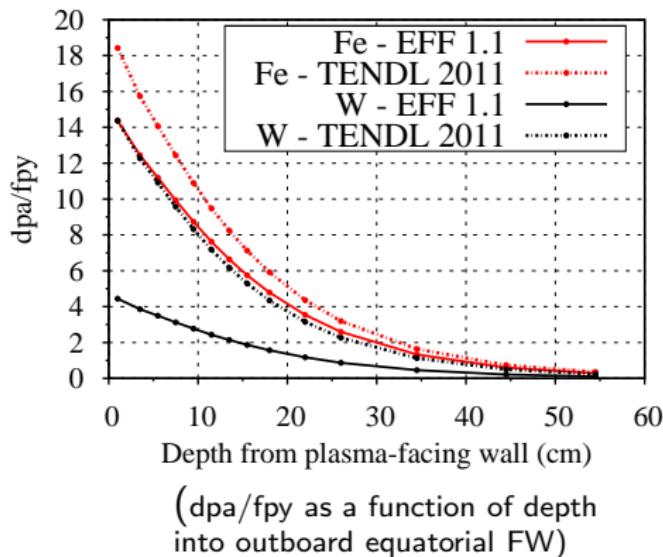
1. dpa: variation with material

- Comparison between W and Fe in FW armour regions



- dpa/fpy in W is $\sim 1/3$ of that in Fe (Nuclear data dependent...)

- ... results from dpa calculations are very sensitive to input reaction-cross-section data



- The newly developed inventory code **FISPACT-II** can calculate dpa values directly from neutron spectra
- Calculations using the latest nuclear data libraries (TENDL-2011) reveal significantly different dpa values to previous results obtained from NJOY using the EFF 1.1 library
- For example, the exposure measured as dpa/fpy in pure W has risen by a factor of 3 in the 2 cm FW armour

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2. Inventory calculations

FISPACT:

- calculates the time-evolution of composition by solving a set of coupled differential equations \forall possible nuclides N_i :

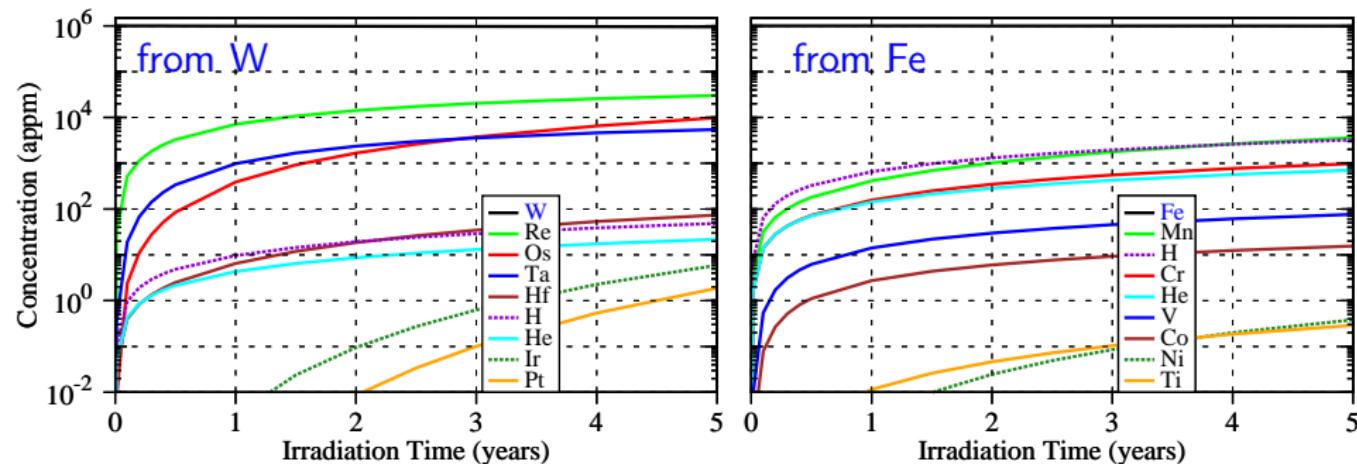
The Bateman equations

$$\frac{dN_i}{dt} = \underbrace{-N_i(\lambda_i + \sigma_i\phi)}_{\text{loss}} + \sum_{j \neq i} \underbrace{N_j(\lambda_{ji} + \sigma_{ji}\phi)}_{\text{creation}}$$

- a database of reaction cross sections ('European Activation File' – EAF) is collapsed with the neutron energy spectra $\rightarrow \sigma_i, \sigma_{ij}$
- EAF also provides decay constants λ_i, λ_{ij}
- fluxes ϕ from neutronics (**MCNP**)

2. Transmutation example

- Pure W and Fe under outboard equatorial FW armour flux for 5 fpy

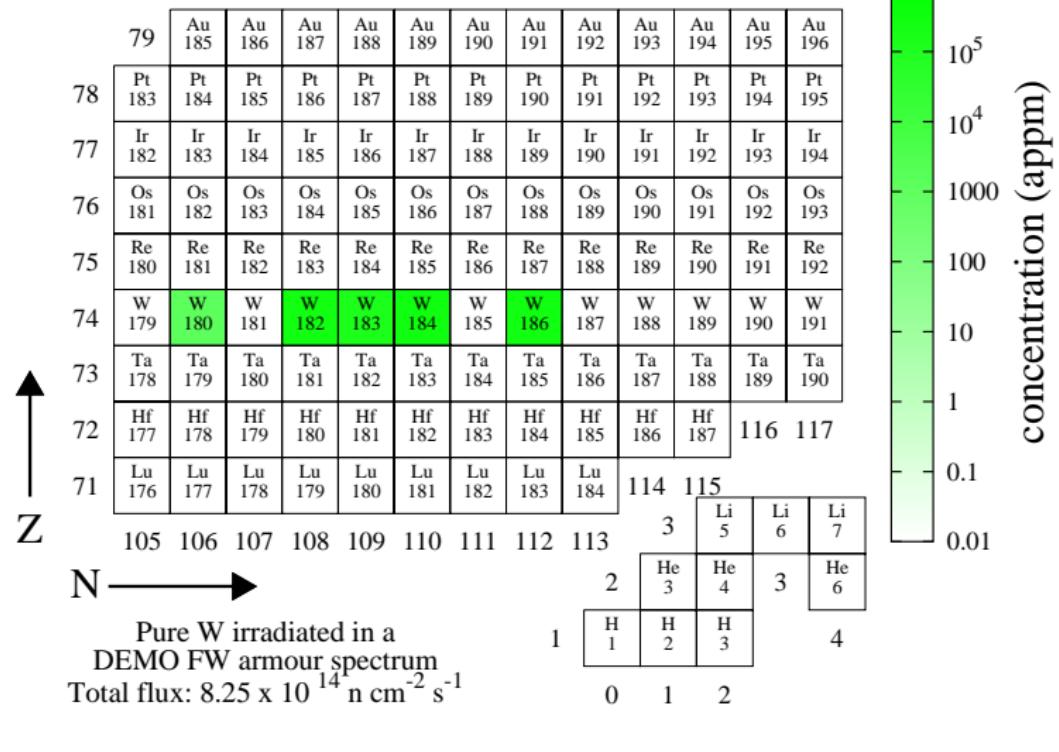


- Metal impurities build-up over time
 - primarily Re, Os, Ta in W
 - Mn and Cr from Fe
- Helium and hydrogen are also produced
 - gas production is very low in W ($\sim \times 10$ less than in Fe)

M.R. Gilbert and J.-Ch. Sublet, *Nuclear Fusion* 51 (2011) 043005

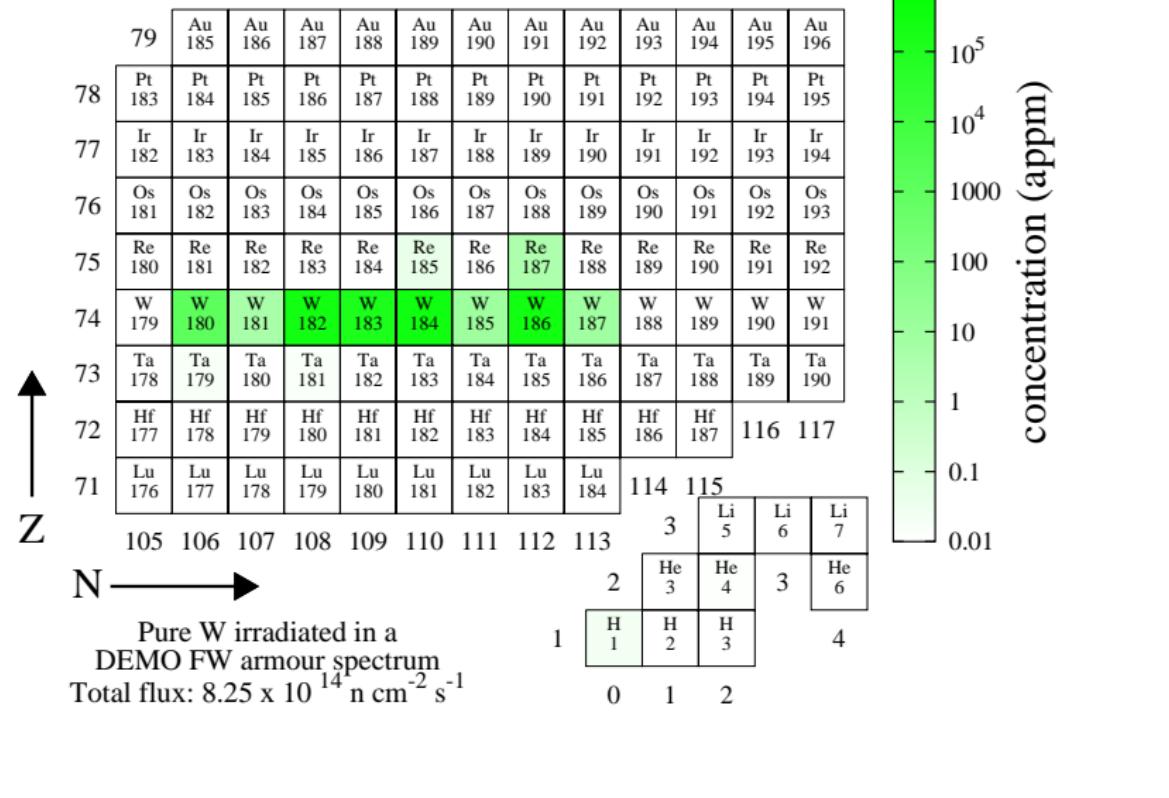
2. W transmutation: 5 fpy FW armour

Time: 0.000 seconds



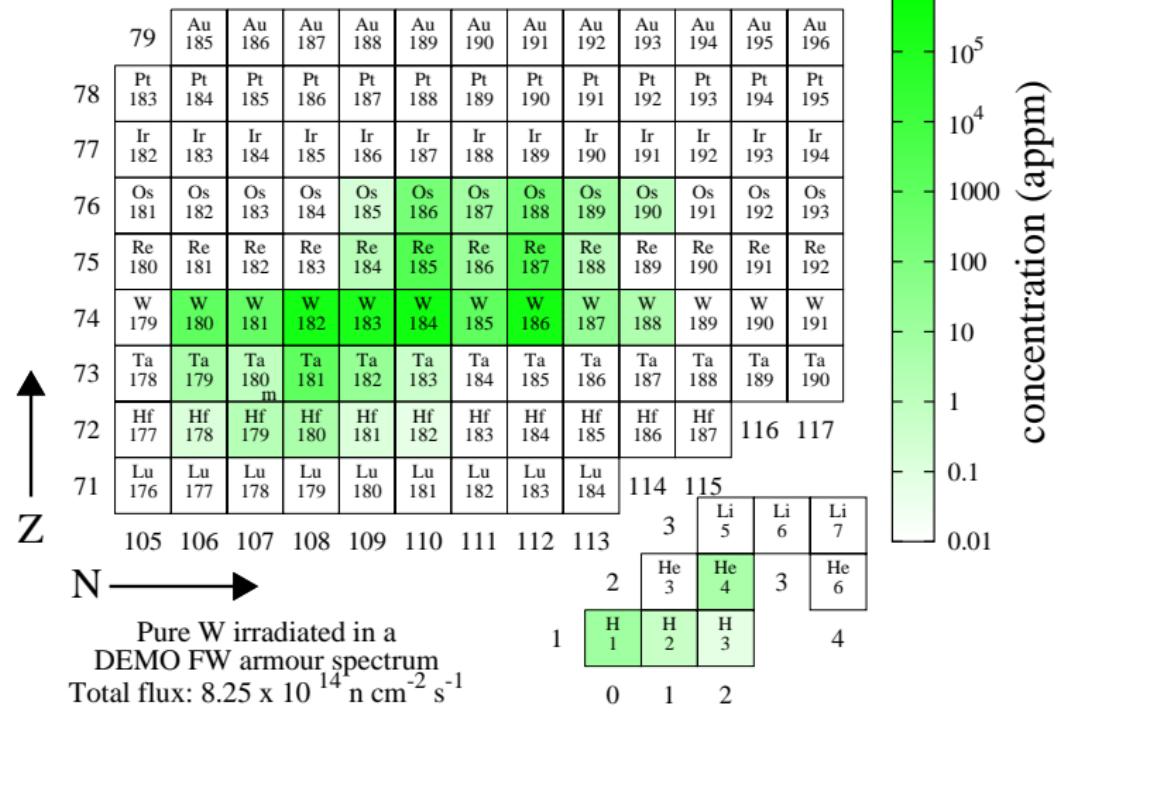
2. W transmutation: 5 fpy FW armour

Time: 1.000 day



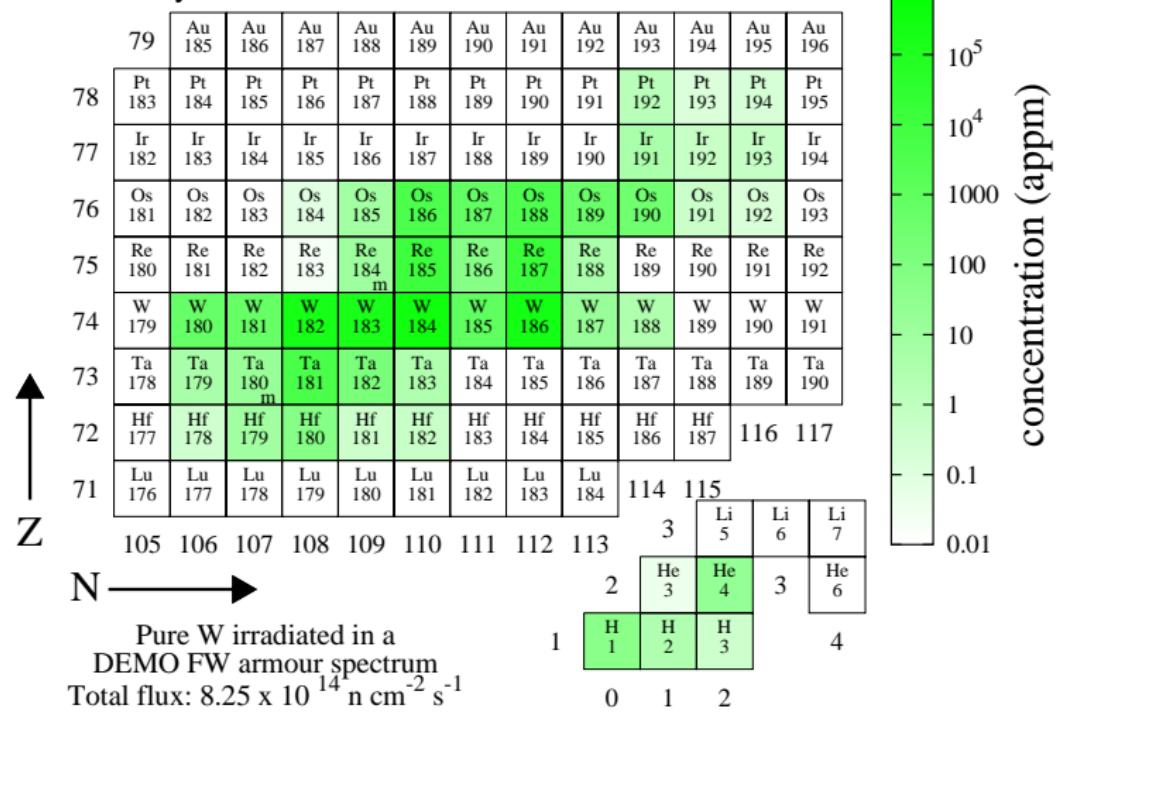
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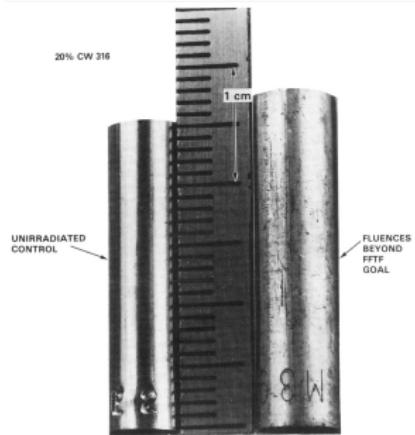
Time: 1.016 years



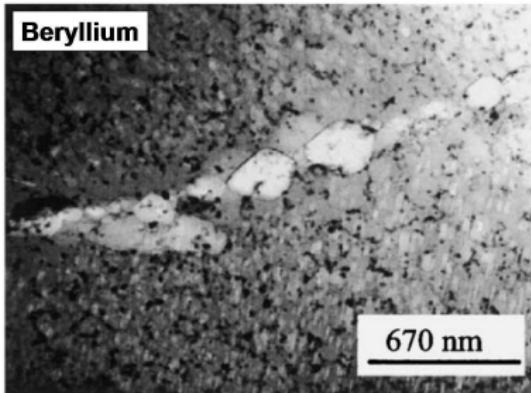
2. W transmutation: 5 fpy FW armour

Time: 5.000 years





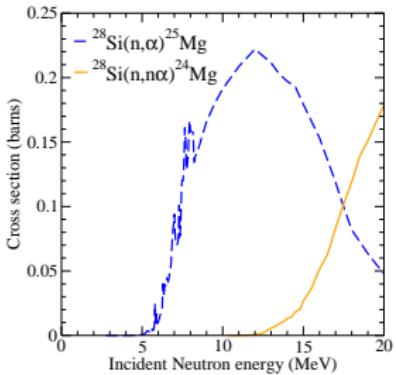
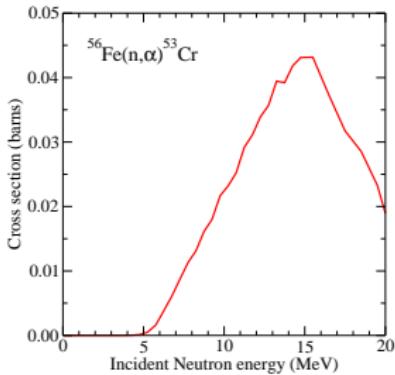
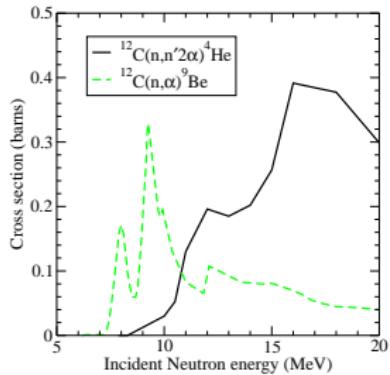
- Transmutant helium can accumulate in pre-existing cracks and voids – swelling
- Helium can also migrate to grain boundaries (GBs) leading to embrittlement
- Particular problem for fusion because of the generally higher neutron energies – many of the helium-producing reactions have thresholds



V.P. Chakin, Z. Ye Ostrovsky
J. Nucl. Mater. **307-311**
(2002) 657

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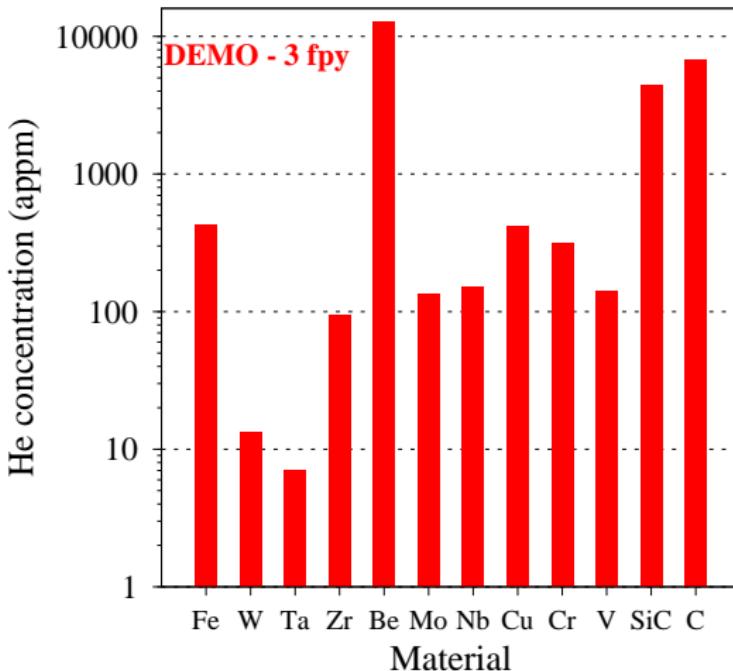
Aside: Motivation for quantifying He production



- Transmutant helium can accumulate in pre-existing cracks and voids – swelling
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2. He production

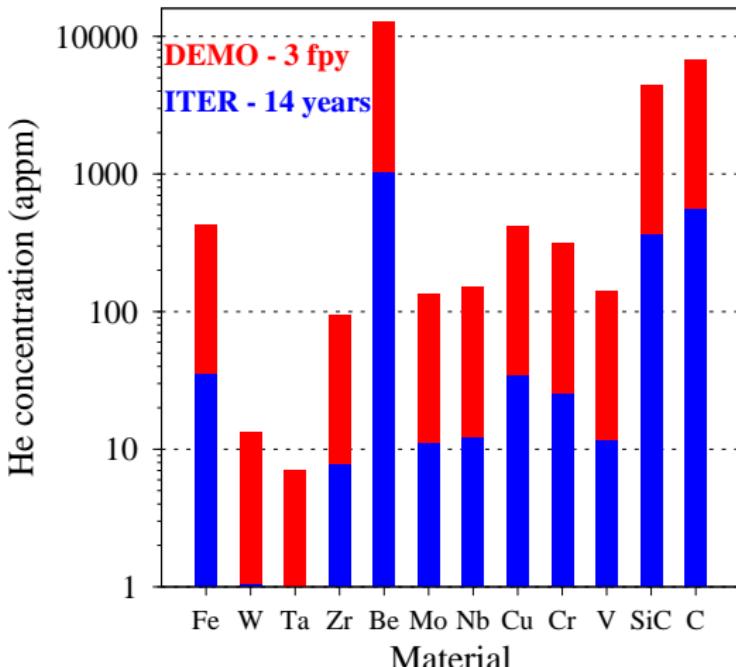
- Material comparison under identical conditions
- 3 fpy under outboard equatorial FW armour irradiation:



- He production highest in Be (~ 4300 appm/fpy)
- More than an order of magnitude lower in Fe (~ 140 appm/fpy)
- Only ~ 4 appm/fpy in W

2. He production

- Material comparison under identical conditions
- 3 fpy under outboard equatorial FW armour irradiation:



- He production highest in Be (~ 4300 appm/fpy)
- More than an order of magnitude lower in Fe (~ 140 appm/fpy)
- Only ~ 4 appm/fpy in W
- concentrations significantly higher than predicted for full-lifetime of ITER FW (with approximate campaign timing)

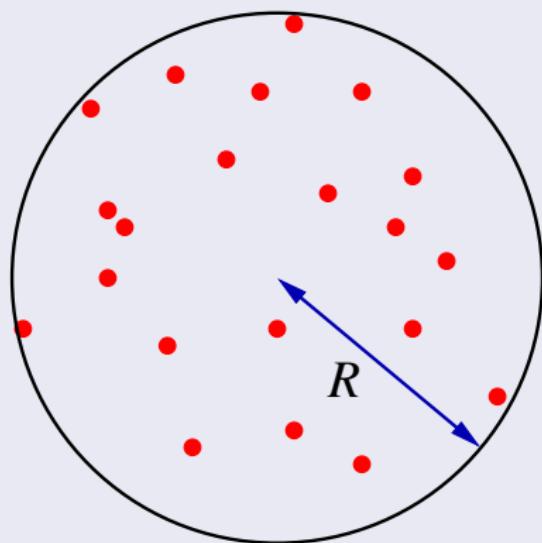
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3. Modelling: He embrittlement of GBs

Simple modelling of grain boundary (GB) failure

1. Number of He atoms in spherical grain:

$$N_{\text{He}} \approx \frac{4}{3}\pi R^3 n G_{\text{He}}$$



Assumptions:

- All helium atoms produced migrate to grain boundary
 - ▶ traps and obstacles neglected
 - ▶ most valid for small grains

G_{He} = bulk concentration
(from inventory calcs.)

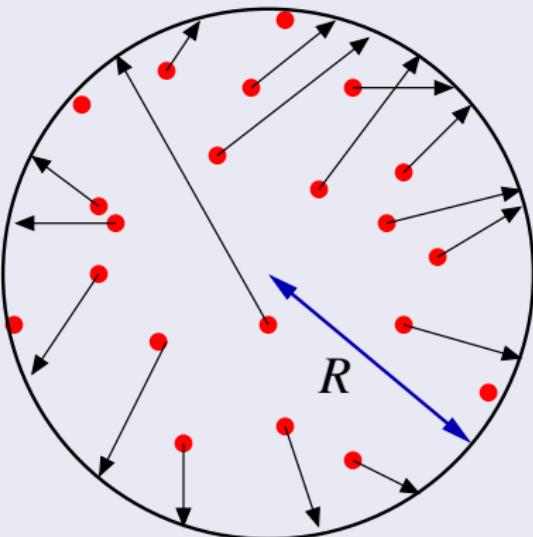
n = atom density

3. Modelling: He embrittlement of GBs

Simple modelling of grain boundary (GB) failure

2. All He atoms move to GB: \therefore surface total \equiv bulk total

$$4\pi R^2 \nu_{\text{He}} = \frac{4}{3}\pi R^3 n G_{\text{He}} \Rightarrow \nu_{\text{He}} = \frac{R}{3} n G_{\text{He}}$$



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G_{He} = bulk concentration
(from inventory calcs.)

ν_{He} = surface density

3. Modelling: He embrittlement of GBs

Simple modelling of grain boundary (GB) failure

3. Assume GBs destabilized when E of solute He equals E of surface:

$$E_{\text{He}}^{\text{sol}} \nu_{\text{He}}^c \approx 2\varepsilon_{\text{surf}}$$

Material	He solution energy (eV)* – $E_{\text{He}}^{\text{sol}}$	Surface energy (Jm ⁻²)* – $\varepsilon_{\text{surf}}$	Critical He conc. at GBs (cm ⁻²) – ν_{He}^c
Fe	4.34	2.4	6.90×10^{14}
Mo	4.65	3.0	8.05×10^{14}
Ta	4.82	3.0	7.77×10^{14}
W	4.77	3.5	9.16×10^{14}
Be	3.46	2.2	7.94×10^{14}
SiC	1.50 [†]	2.5	2.08×10^{15}

* Estimates taken from: F. Willaime and C. C. Fu, 2006, *Mater. Res. Soc. Symp.*, **981** 0981-JJ05-04, M. G. Ganchenkova *et al.*, 2009, *J. Nucl. Mater.*, **386–388** 79–81, L. Vitos *et al.*, 1998, *Surf. Sci.*, **411** 186–202, Yu M. Koroteev *et al.*, 2009, *Phys. Solid State*, **51** 1600–1607, and S. C. Middleburgh and R. W. Grimes, 2011, *Acta Mater.*, **59** 7095–7103

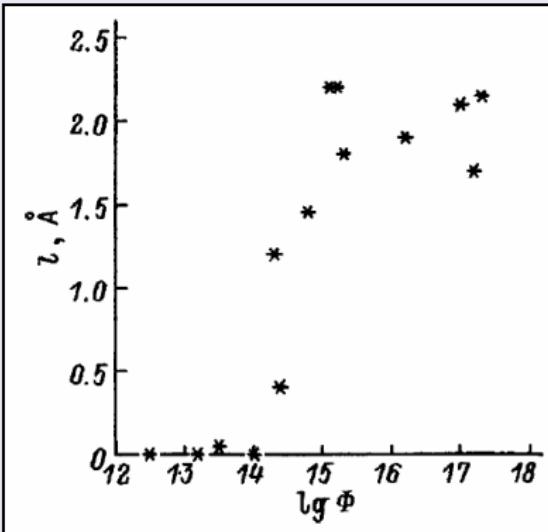
[†] Energy for He interstitial surrounded by Si atoms – R. M. Van Ginhoven *et al.*, 2006, *J. Nucl. Mater.*, **51** 348

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Simple modelling of grain boundary (GB) failure

3. Assume GBs destabilized when E of solute He equals E of surface:

$$E_{\text{He}}^{\text{sol}} \nu_{\text{He}}^c \approx 2\varepsilon_{\text{surf}}$$



- Experimental confirmation:
 - ▶ Helium irradiated W bicrystals
 - ▶ Expansion of grain boundaries at He fluence of 10^{14} – 10^{15} ions cm^{-2}
 - ▶ our ν_{He}^c value: 7.51×10^{14}

Gerasimenko, Mikhaĭlovskiĭ,
Neklyudov, Parkhomenko, and
Velikodnaya
Tech. Phys. **43** (1998) 803

3. Modelling: He embrittlement of GBs

Simple modelling of grain boundary (GB) failure

4. Critical bulk He concentration:

$$G_{\text{He}}^c = \frac{3}{Rn} \nu_{\text{He}}^c$$

Material	ν_{He}^c (cm $^{-2}$)	n (cm $^{-3}$)	G_{He}^c (appm)
Fe	6.90×10^{14}	8.5×10^{22}	488.0
Mo	8.05×10^{14}	6.4×10^{22}	753.2
Ta	7.77×10^{14}	5.5×10^{22}	841.3
W	9.16×10^{14}	6.3×10^{22}	871.5
Be	7.94×10^{14}	1.2×10^{23}	385.2
SiC	2.08×10^{15}	4.7×10^{22}	2645.6

- Assumed Grain size of $R = 0.5\mu\text{m}$
- G_{He}^c varies linearly with $1/R$

3. Critical lifetimes for GB embrittlement by He

- Critical embrittlement lifetimes estimated using FISPACT

Material	G_{He}^c (appm)	Critical GB embrittlement lifetimes t_{He}^c for DEMO			
		Outboard Equatorial FW	Polar FW	Equatorial blanket 17-19 cm	Shielded divertor armour
Fe	488.0	4 years	7 years	18 years	78 years
Mo	753.2	18 years	36 years	114 years	420 years
Ta	841.3	216 years	300+ years	300+ years	300+ years
W	871.5	300+ years	300+ years	300+ years	300+ years
Be	385.2	1 month	2 months	4 months	1.5 years
SiC*	2645.6	1.8 years	3.5 years	9.5 years	41 years

- Wide variation in lifetimes between different materials and for the same material as a function of position
- Be has very short expected lifetimes
- This type of failure probably won't occur in W (or Ta)

- An integrated model of neutron-irradiation-induced changes in material properties for DEMO:
- 1. Neutron-transport simulations of a fusion reactor model:
 - ▶ wide variation in exposure with depth and position - even within the same components
- 2. Inventory calculations:
 - ▶ the variation in irradiation environment creates large differences in the transmutation or burn-up rates of materials
 - ▶ He production rates are strongly dependent on material
- 3. Simple modelling of He-induced grain-boundary embrittlement suggests that some materials could fail on relatively short timescales (Be in particular)

Future

- Fully heterogenous reactor models could predict very different irradiation conditions
- The GB failure model needs to fully account for the traps and migration barriers for He
 - ▶ lifetimes could be increased in a more complete model
- Integration of other predictive techniques:
 - ▶ e.g. swelling-induced stresses leading to fracture, changes in strength due to transmutation impurities, etc.