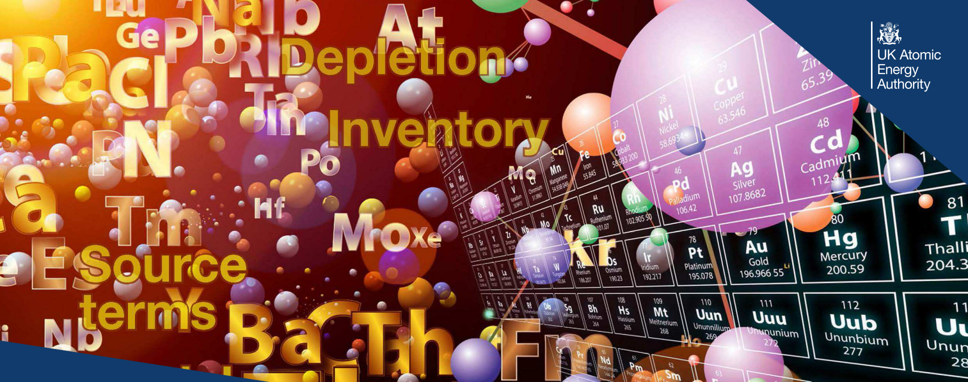

UK Atomic Energy Authority

FISPACT-II

Self-shielding & spatial variation case study: tungsten in a fusion device

Mark Gilbert
United Kingdom Atomic Energy Authority

FISPACT-II workshop

October 23-25, 2019, Manchester

Research Councils UK Energy For a Low Carbon Future
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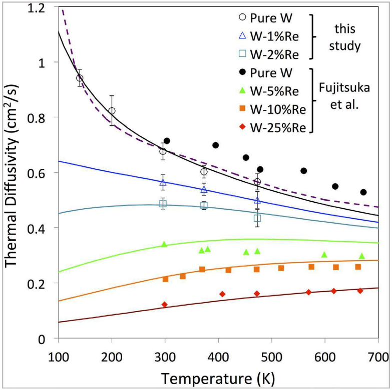
Introduction

- A key feature of tunsten's (W) desirability as an armour material is its good thermal conductivity
- But recent experiments & modelling demonstrate that the thermal properties of W can be changed by the addition of Rhenium (Re)
- Accurate quantification of Re production via transmutation in W is vital to predict performance
- But must rely on simulations to provide predictions to design engineers



Hofmann *et al.*, *Sci. Rep.* **5** (2015) 16042

- Re reduces thermal diffusivity of W

Introduction

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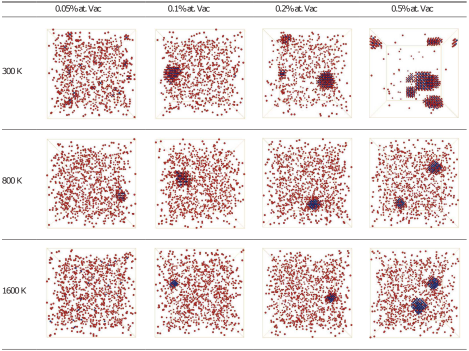
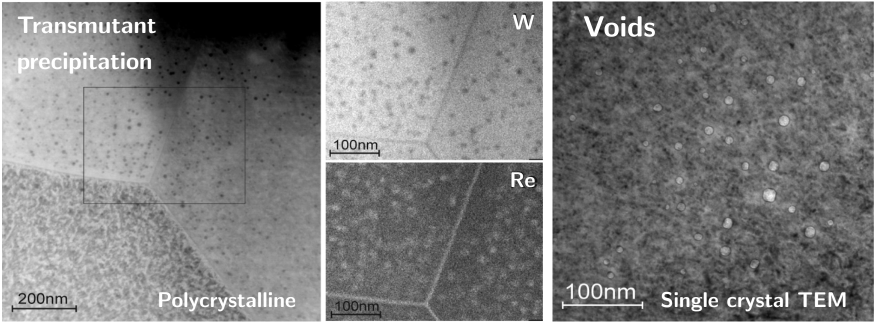


Wrobel *et al.*, *J. Phys.: Condens. Matter* **29** (2017) 145403

- Re forms precipitates in W under irradiation, affecting both thermal and mechanical properties

Motivation for analysis

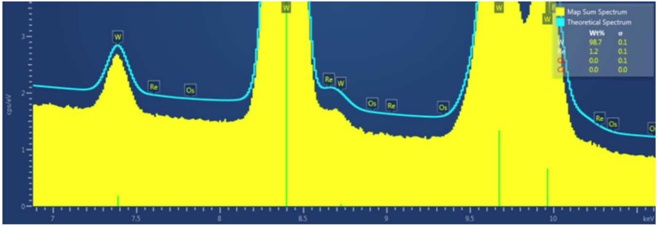
- In W the issue is complicated by the sensitivity of transmutation rates to the local neutron environment
- Predictive simulations are only reliable if the neutron fields are properly characterised
- As was recently demonstrated in a experimental vs. simulation comparison of Re concentrations in W irradiated at HFR, Petten (part of the EXTREMAT-II project)



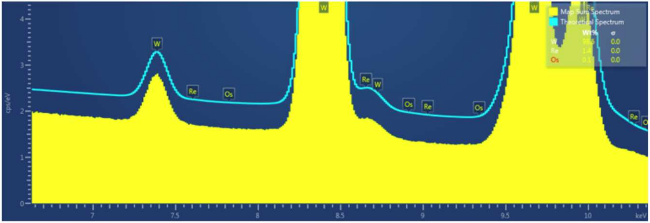
Klimenkov *et al.*
Nucl. Mater. Ene. **9** (2016) 480-483

Motivation for analysis

- Energy Dispersive X-ray (EDX) measurements of irradiated W samples indicated 1.2-1.4% Re ...



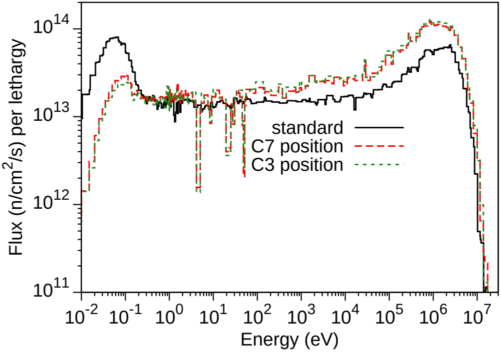
Petten Single Crystal (1.2wt% Re measured)



Petten Polycrystalline (1.4wt% Re measured)

Motivation for analysis

- ... but FISPACT-II calculations performed with standard simulated spectrum for HFR over-predicted Re production
  - $\sim 4\%$
- New neutron transport simulations taking into account local environment, including other nearby experiments (other W & Gd thermal absorbers), produced spectra with important differences
  - lower thermal component & resonance self-shielding flux depletions



Irradiation scenario

- W irradiated under EXTREMAT-II in 2008 & 2009
- Target of 282 days of irradiation (10 cycles), but in fact only irradiated in 8 cycles & in two different positions

Position	Cycle	EFPD	Start date	End date
C7	08-May	30.72	22-May-08	22-Jun-08
	08-Jun	29.71	28-Jun-08	28-Jul-08
C3	09-Jan	27.69	12-Feb-09	12-Mar-09
	09-Feb	24.99	01-Apr-09	26-Apr-09
	09-Mar	30.77	29-Apr-09	30-May-09
	09-Apr	24.71	02-Jun-09	27-Jun-09
	09-May	17.61	30-Jun-09	18-Jul-09
	09-Jun	22.06	17-Aug-09	08-Sep-09
Total		208.26		

EFPD effective full power days

FISPACT-II input

```
...
GETXS 0 << first spectrum >>
GETDECAY 0
FISPACT
* W 5-year transmute
MASS 1 1
W 100.0
...
FLUX 6.61372910E+14
ATOMS
TIME 30.72 DAYS ATOMS
FLUX 0.0
TIME 6 DAYS ATOMS
FLUX 6.61372910E+14
TIME 29.71 DAYS ATOMS
FLUX 0.0
TIME 199 DAYS ATOMS << time between first and second phase >>
GETXS 0 << second spectrum >>
FLUX 6.83278750E+14
TIME 27.69 DAYS ATOMS
FLUX 0.0
TIME 20 DAYS ATOMS
FLUX 6.83278750E+14
TIME 24.99 DAYS ATOMS
FLUX 0.0
TIME 3 DAYS ATOMS
FLUX 6.83278750E+14
TIME 30.77 DAYS ATOMS
FLUX 0.0
TIME 3 DAYS ATOMS
FLUX 6.83278750E+14
TIME 24.71 DAYS ATOMS
FLUX 0.0
TIME 3 DAYS ATOMS
FLUX 6.83278750E+14
TIME 17.61 DAYS ATOMS
FLUX 0.0
TIME 30 DAYS ATOMS
FLUX 6.83278750E+14
TIME 22.06 DAYS ATOMS
FLUX 0.0
ZERO
TIME 6 YEARS << 8 September 2009 to 8 September 2015 >>
ATOMS
...
```

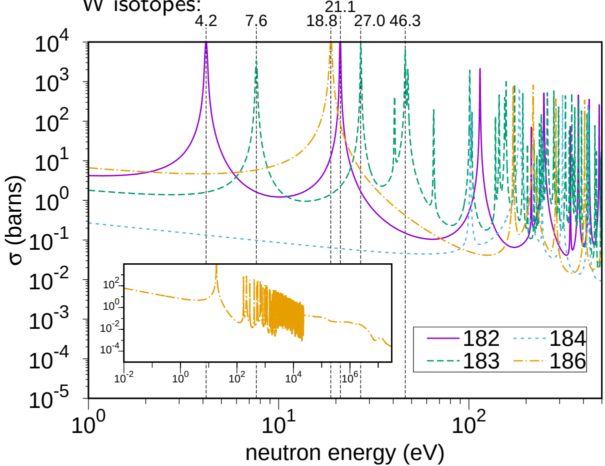
- Full complexity simulated in FISPACT-II - including change of location (two separate `COLLAPX` files created using the two spectra and loaded sequentially)

Motivation for analysis

- 1.45 wt% Re predicted using correctly calculated spectrum and properly accounted for self-shielding
  - good agreement with 1.2-1.4% measured in experiment
- demonstrated the importance of included self-shielding in calculations and also that subtle changes in neutron fields can have dramatic influence on transmutation rates

Nuclear interactions

- Why is transmutation in W sensitive to neutron field shape?
- Reaction cross sections (xs) σ for (n,γ) neutron-capture channels on W isotopes:



^{182}W – 26.5 atm.%

^{183}W – 14.31

^{184}W – 30.64

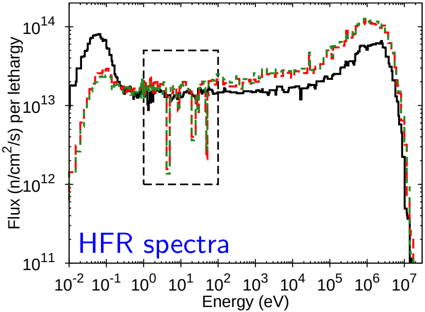
^{186}W – 28.43

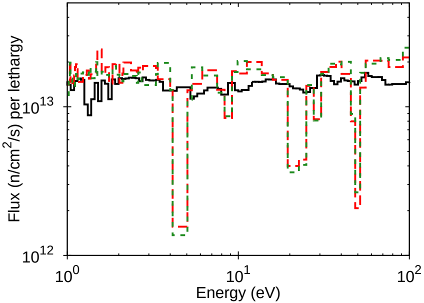
- small changes in the neutron fluxes at the energy of "giant" resonances can dramatically alter reaction rates (RRs)
- & xs high in thermal energy range ($\sim$ 0.025 eV)

Re production rates are controlled by RRs of (n,γ) on ^{186}W & ^{184}W, as well as (n,2n) neutron multiplication on ^{186}W

Influences on spectrum

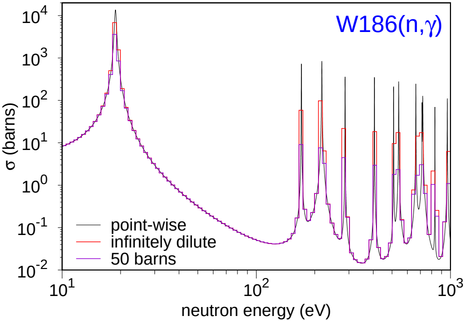
- The neutron spectrum in the energy regions of the giant resonances below ∼30 eV can be altered by increased neutron absorption and moderation ...
  - perhaps due to the local presence of water or other moderator
- ... and also by self-shielding
  - where the giant resonances absorb many of the slowing neutrons causing localised flux "depletions"

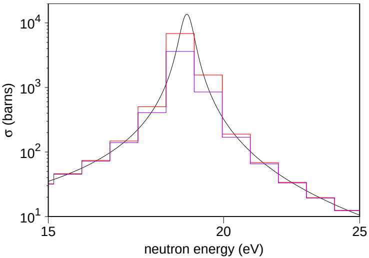




Self-shielding in simulations

- FISPACT-II includes the necessary high-resolution nuclear data to correctly model the self-shielding "dilutions" associated with giant resonances



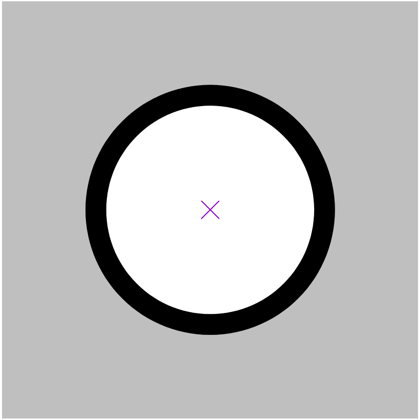


- But the neutron transport simulations must also have sufficient resolution in:
  - the energy grid of the statistical tallies to capture influence of resonances
  - & the geometry to capture local variation in thermal & fast energy regions

http://fispact.ukaea.uk

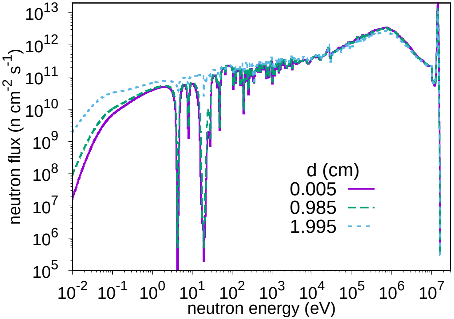
Neutron field simulations

- Variation in Re production studied in high spatial resolution, but in a simplified geometry
  – easier to get good statistical accuracy
- Spherical W shell 2cm thick (black), radius 10-12 cm, surrounding a 14 MeV neutron source
- & surrounded by a 80-20% Steel-water mix (grey)
- neutron flux spectrum recorded separately in every 0.1 mm layer of the W during an (MCNP) neutron simulation of 10^{10} histories
  - in a bin structure containing 709 energy groups (same as nuclear reaction data)

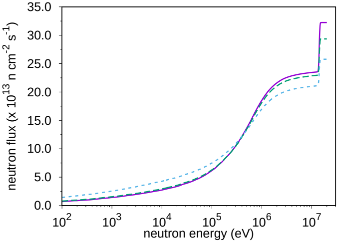


Neutron spectra results

- Even in first 0.1 mm the flux depletions due to the giant resonances are present
  - suggesting that self-shielding occurs at all depths because neutron backscattering populates all neutron energies
- Flux depletions are reduced in W layers close to the moderator & thermal component of spectrum is higher
  - potential change in transmutation behaviour



- 20% drop in total flux across 2 cm depth



Transmutation Calculations

- Simulations with FISPACT-II:

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

  - using TENDL nuclear reaction data in high energy-grid resolution format (709 groups)
    - particularly in lower resolved resonance range from 0.1 to 10 eV
    - & in fast neutron range (5-30 MeV) for accurate reaction rates (RRs) of threshold reactions
- 2-year continuous irradiation (2 "full-power years" [fpy]) simulated
- Neutron flux results scaled to produce equivalent 2 MW/m^2 on inner, plasma-facing surface of W shell
- Appropriate, probability-table-derived self-shielding factors (SSFs) applied to neutron capture reactions on W isotopes to account for self-shielding and cross section dilutions

FISPACT-II input

- To correctly account for self-shielding in all isotopes of W
  - During reading of cross section data ("collapse"):

```
PROBTABLE 0 1
SSFCHOOSE 1 0 W
SSFMASS 1.0 1
W 100.0
GETXS 1 709
```

- `PROBTABLE <<option>> <<partials>>`
  - turns on self-shielding corrections using probability tables
  - data tables provided in `prob_tab` entry of `files`
  - `<<option>>`:
    - if 1 then apply multiplication factors
    - if 0 (default) replace cross sections

FISPACT-II input

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```
PROBTABLE 0 1
SSFCHOOSE 1 0 W
SSFMASS 1.0 1
W 100.0
GETXS 1 709
```

- `PROBTABLE <<option>> <<partials>>`
  - `<<partials>>`:
    - if 0 then calculate corrections based on total cross sections
    - if 1 (default) then calculated corrections for each macro-partial
- in general the different options will yield similar results – use defaults if in doubt

FISPACT-II input

- To correctly account for self-shielding in all isotopes of W
  - During reading of cross section data ("collapse"):

```
PROBTABLE 0 1
SSFCHOOSE 1 0 W
SSFMASS 1.0 1
W 100.0
GETXS 1 709
```

- `SSFCHOOSE <<n>> <<print>>`
  - selects which `<<n>>` elements (or nuclides) to self-shield
    - if elements then all natural isotopes of each are considered
  - `<<print>>`:
    - if 0 then print table of corrected total cross sections
    - if 1 then print energy-dependent breakdown of corrections for each cross section

FISPACT-II input

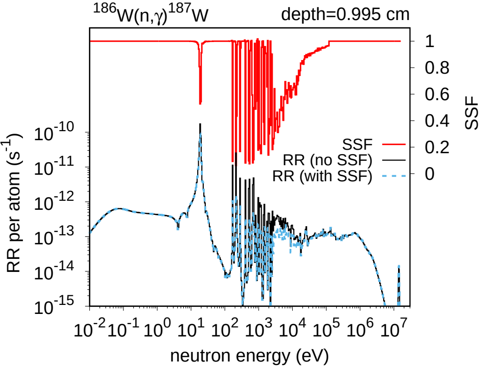
- To correctly account for self-shielding in all isotopes of W
  - During reading of cross section data (“collapse”):

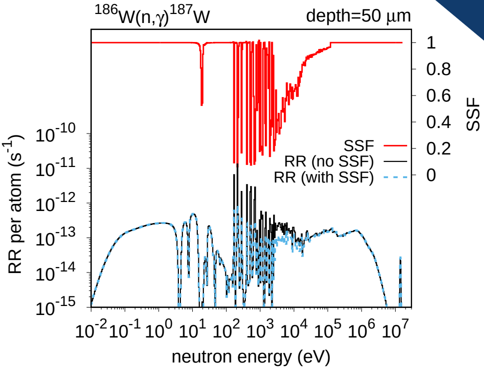
```
PROBTABLE 0 1
SSFCHOOSE 1 0 W
SSFMASS 1.0 1
W 100.0
GETXS 1 709
```

- `SSFMASS <<mass>> <<n>>`
  - specifies which composition should be used when calculating self-shielding corrections
  - equivalent to `MASS` keyword in main inventory
  - similarly, `SSFFUEL` is an alternative and equivalent to `FUEL`

Reaction rate (RR) corrections

- Probability Table (PT) SSFs used to account for dilution effects associated with both resolved and un-resolved ($>\sim$ 20 keV) resonances





- final 0.1 mm of W
- total SSF: 0.64
- giant resonance dominates RR of ^{186}W (n,γ) (70% of RR)

- first 0.1 mm of W
- total SSF: 0.55
- minor contribution from giant resonance

Plots derived from `extract_xs_endf` utility

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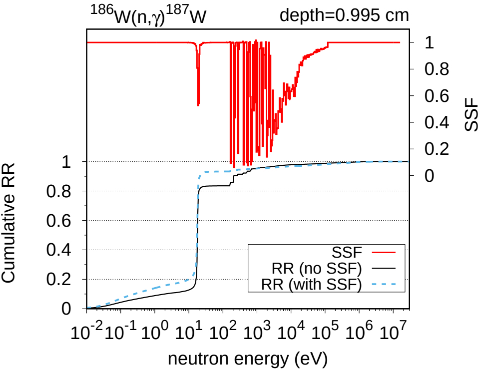

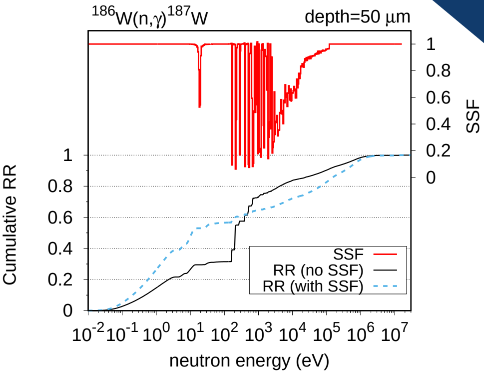

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Plots derived from extract_xs_endf utility

FISPACT-II output

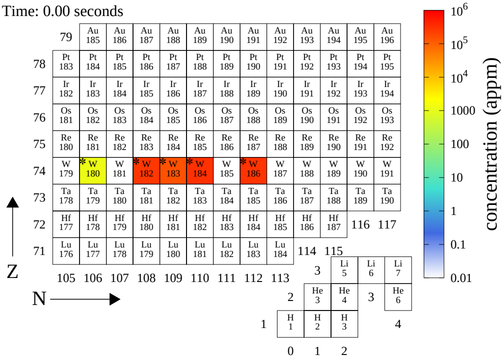
- example output summary of probability table changes to cross sections

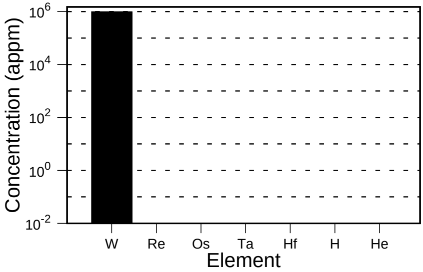
parent nuclide	daughter nuclide	mt	cal-mt	old sigma barns	new sigma barns	self shielding factor (%)
W 180	W 180	2	2	7.10713E+00	6.97849E+00	98.19
W 180	W 181	102	101	1.42897E+00	1.31879E+00	92.29
W 182	W 182	2	2	7.08710E+00	5.80090E+00	81.85
W 182	W 183	102	101	3.23138E-01	1.63337E-01	50.55
W 182	W 183m	102	101	1.84613E-03	1.57691E-03	85.42
W 183	Hf180	107	101	1.32471E-04	1.32355E-04	99.91
W 183	Hf180m	107	101	1.26413E-05	1.26413E-05	100.00
W 183	W 183	2	2	6.22868E+00	5.43190E+00	87.21
W 183	W 184	102	101	6.75776E-01	3.56673E-01	52.78
W 184	W 184	2	2	6.54344E+00	5.67783E+00	86.77
W 184	W 185	102	101	1.37662E-01	8.17256E-02	59.37
W 184	W 185m	102	101	1.65598E-03	1.48305E-03	89.56
W 186	W 186	2	2	7.08482E+00	5.96675E+00	84.22
W 186	W 187	102	101	2.73553E-01	1.52878E-01	55.89

- in this case the (n,γ) (MT=102) channels on the main W isotopes are reduced by nearly 50%

Inventory evolution example

- Evolution in time of compositions from FISPACT-II output
- nuclide picture shown on a "chart of the nuclides"
- 2-year irradiation under spectrum predicted at centre of W shell:





- Large spread of isotopes produced – increasing as a function of time as longer & longer reaction chains are created

m – concentration dominated by metastable state of isotope

appm - atomic parts per million
* nuclide present in input composition

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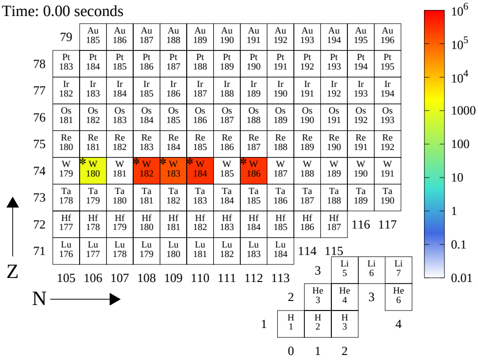

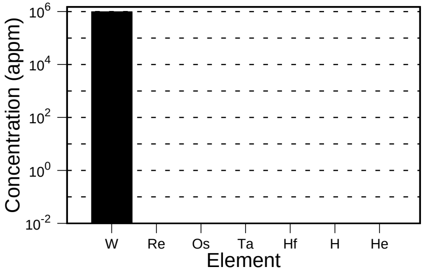

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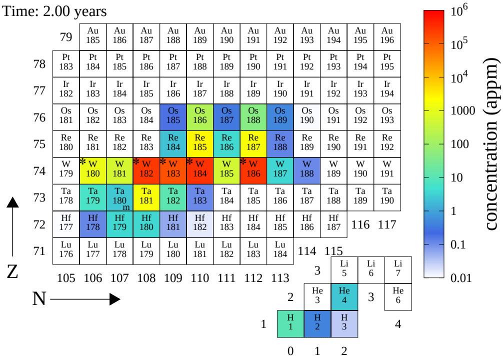

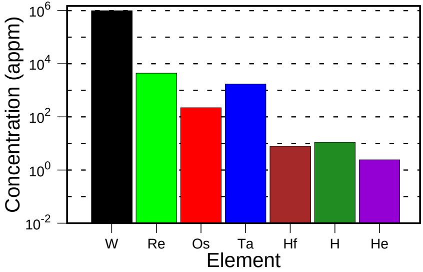

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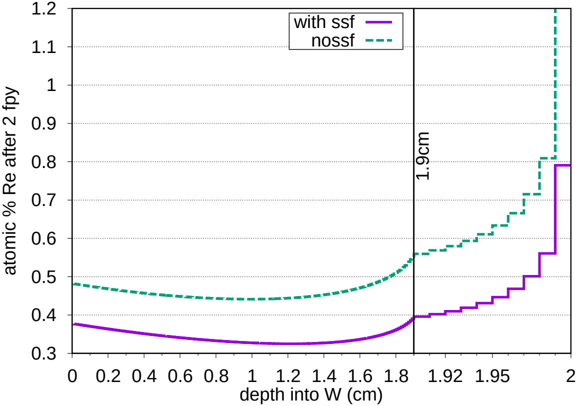
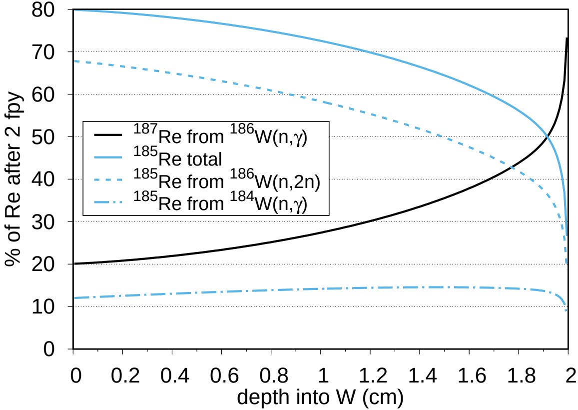
Re production results



- PT-based SSFs are important (avoiding a 20-50% over-prediction)
- But the spatial heterogeneity is much more significant

- factor 2-3 increase in Re production near moderator, despite overall (20%) drop in flux
- results show that standard "averaging" of neutron fields over large volumes would produce a misleading picture (average is only 0.35 atm%)

Re production routes (reaction pathways)

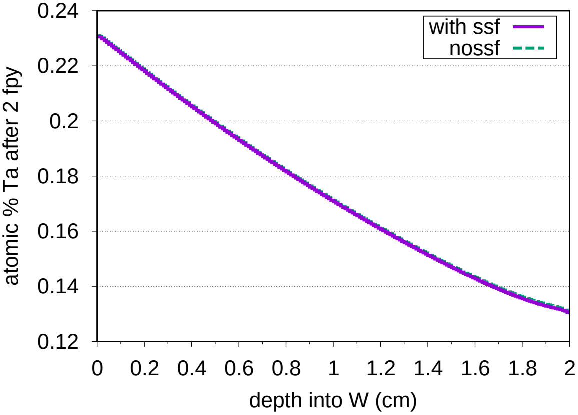


- Stable ^{185}Re & ^{187}Re are dominate Re isotopes ($\sim$100% of total) produced
- Their proportion (and main production routes) change with depth

- Near the front ^{185}Re dominates & is mainly produced from the threshold (n,2n) reaction on ^{186}W, due to the relatively hard neutron spectrum
- At the back of the W ^{187}Re, produced via (n,γ) on ^{186}W, becomes dominant in the last 1-2 mm due to an increase in backscattered, low-energy neutrons – softer neutron spectrum & dominance of giant resonances

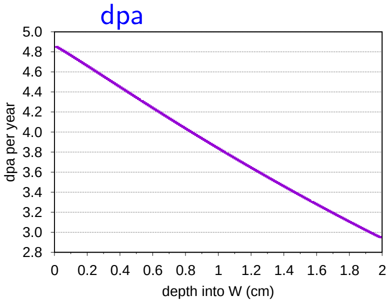
Effect on other quantities: Tantalum production

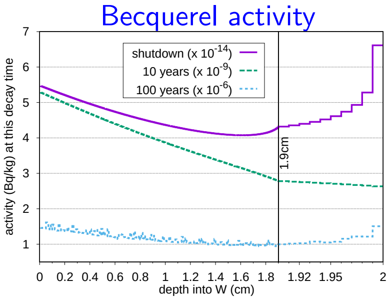
- Ta production from same modelling of a 2-year irradiation:



- Production dominated by (n,2n) reaction on ^{182}Ta ($>$ 90%)
- RR of this threshold reaction varies only with flux of high-energy neutrons
  - backscattering from moderator and self-shielding has little impact

Effect on other quantities: dpa & activity

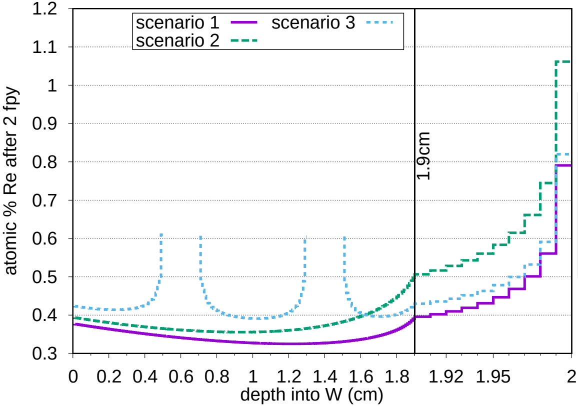


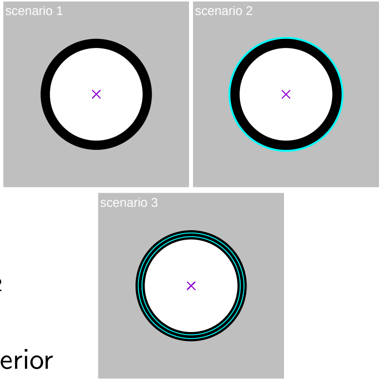


- displacements per atom (dpa) dose follows moderation in fast flux with depth
- Activity (during cooling after 2-year irradiation) picture more complex:
  - at short decay times – W isotopes dominate (moderator geometry important)
  - medium times – Ta isotopes dominate (only fast-flux moderation matters)
  - longer times – ^{186}Re contributes (some influence of geometry)

More complex scenarios

- Re production after 2-years in different geometries:



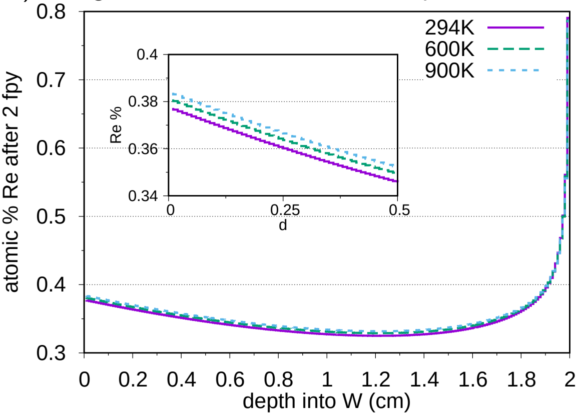


- separate water channels (exterior or interior to W shell) enhance local variation

$\Rightarrow$ correct modelling of heterogeneity is crucial

Temperature effects

- Re production after 2-years at different temperatures (scenario 1) using nuclear libraries with temperature corrections:



- Doppler broadening of resonances with temperature increases neutron-capture reaction rates & hence Re production
- But effect is relatively minor in these simulations

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Summary

- Standard practice of simulating compositional changes due to transmutation using neutron spectra (fields) averaged (homogenized) over large reactor-model volumes can lead to misleading (wrong) predictions for W
- Fine length-scale simulations of W reveal that there is a large sensitivity in Re production due to the local environment
  - caused by subtle changes in neutron spectrum due to moderation and backscattering
- The heterogeneity (with geometry) can be even more significant than self-shielding of giant capture resonances in W
  - but self-shielding nonetheless needs to be accounted for
- FISPACT-II can correct for self-shielding but still relies on realistically calculated (neutron) irradiation fields

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