Integrated computational study of material lifetime in a fusion reactor environment

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• The neutrons generated in fusion plasmas bombard the surrounding materials...
  ▶ $\sim 10^{15}$ neutrons cm$^{-2}$ 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
Integrated studies (talk outline)

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1. Neutronics: DEMO model for MCNP

- 2009 model designed using HERCULES\(^1\)
- 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

\(^1\)Pampin 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 $8.25 \times 10^{14}$ n cm$^{-2}$ s$^{-1}$
  - In final 5 cm of blanket drops to $3.90 \times 10^{13}$ n cm$^{-2}$ s$^{-1}$
  - In vessel walls it is only $1.38 \times 10^{12}$ n cm$^{-2}$ s$^{-1}$
- Variation is complex, so standard practice is to calculate integrated quantity $\rightarrow$ 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)

\[ dpa \text{ per second} = \sum_i N_g \phi_i \sigma_i^{dpa} \]

- shows the variation in “exposure” with position

- dpa/fpy in Fe in FW armour is \( \sim 3 \) 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

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

Damage varies with temperature for same dpa

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...

**Bar Graph**

- dpa/fpy
- Flux

**Diagram**

- Poloidal positions labeled A to M
- Equivalent flux (n cm\(^{-2}\) s\(^{-1}\))
- Plasma region

\(\text{dpa/fpy in Fe} \times 10^{14}\) equivalent flux (n cm\(^{-2}\) s\(^{-1}\))
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

- \[ \text{dpa/fpy in W is } \sim 1/3 \text{ of that in Fe (Nuclear data dependent...)} \]
• ... 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 $N_i$:

\[
\frac{dN_i}{dt} = -N_i(\lambda_i + \sigma_i \phi) + \sum_{j \neq i} N_j(\lambda_{ji} + \sigma_{ji} \phi)
\]

**The Bateman equations**

- 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 $\lambda_i, \lambda_{ij}$
- fluxes $\phi$ 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)

2. W transmutation: 5 fpy FW armour

Time: 0.000 seconds

Pure W irradiated in a DEMO FW armour spectrum
Total flux: $8.25 \times 10^{14}$ n cm$^{-2}$ s$^{-1}$

appm = atomic parts per million
2. W transmutation: 5 fpy FW armour

Time: 1.000 day

Pure W irradiated in a DEMO FW armour spectrum

Total flux: $8.25 \times 10^{14}$ n cm$^{-2}$ s$^{-1}$

appm = atomic parts per million
2. W transmutation: 5 fpy FW armour

Time: 1.016 years

Pure W irradiated in a DEMO FW armour spectrum

Total flux: $8.25 \times 10^{14} \text{ n cm}^{-2} \text{ s}^{-1}$
2. W transmutation: 5 fpy FW armour

Time: 5.000 years

Pure W irradiated in a DEMO FW armour spectrum
Total flux: $8.25 \times 10^{14}$ n cm$^{-2}$ s$^{-1}$

appm = atomic parts per million
Aside: Motivation for quantifying He production

- 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
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Aside: Motivation for quantifying He production

V.P. Chakin, Z. Ye Ostrovsky
Aside: Motivation for quantifying He production

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- Particular problem for fusion because of the generally higher neutron energies – many of the helium-producing reactions have thresholds

Cross section (barns) vs. Incident Neutron energy (MeV)

1 barn = $10^{-24}$ cm$^2$
2. He production

- Material comparison under identical conditions
- 3 fpy under outboard equatorial FW armour irradiation:
  - He production highest in Be ($\sim 4300$ appm/fpy)
  - More than an order of magnitude lower in Fe ($\sim 140$ appm/fpy)
  - Only $\sim 4$ appm/fpy in W

![He concentration (appm) vs Material](image)
2. He production

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- 3 fpy under outboard equatorial FW armour irradiation:
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  - More than an order of magnitude lower in Fe (\(\sim 140\) appm/fpy)
  - Only \(\sim 4\) appm/fpy in W
  - Concentrations significantly higher than predicted for full-lifetime of ITER FW (with approximate campaign timing)

![He concentration graph](image)
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\[\text{ppm} = \text{atomic parts per million}\]
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

\[ G_{\text{He}} = \text{bulk concentration} \]
\[ n = \text{atom density} \]
3. Modelling: He embrittlement of GBs

Simple modelling of grain boundary (GB) failure

2. All He atoms move to GB: \[ \therefore \text{surface total} \equiv \text{bulk total} \]

\[
4\pi R^2 \nu_{\text{He}} = \frac{4}{3} \pi R^3 n_{G_{\text{He}}} \quad \Rightarrow \quad \nu_{\text{He}} = \frac{R}{3} n_{G_{\text{He}}}
\]

Assumptions:
- All helium atoms produced migrate to grain boundary
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\( G_{\text{He}} = \text{bulk concentration} \)  
\( \nu_{\text{He}} = \text{surface density} \)
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:

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

<table>
<thead>
<tr>
<th>Material</th>
<th>He solution energy (eV) $- E_{\text{He}}^{\text{sol}}$</th>
<th>Surface energy (Jm$^{-2}$) $- \varepsilon_{\text{surf}}$</th>
<th>Critical He conc. at GBs (cm$^{-2}$) $- \nu_{\text{He}}^c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>4.34</td>
<td>2.4</td>
<td>$6.90 \times 10^{14}$</td>
</tr>
<tr>
<td>Mo</td>
<td>4.65</td>
<td>3.0</td>
<td>$8.05 \times 10^{14}$</td>
</tr>
<tr>
<td>Ta</td>
<td>4.82</td>
<td>3.0</td>
<td>$7.77 \times 10^{14}$</td>
</tr>
<tr>
<td>W</td>
<td>4.77</td>
<td>3.5</td>
<td>$9.16 \times 10^{14}$</td>
</tr>
<tr>
<td>Be</td>
<td>3.46</td>
<td>2.2</td>
<td>$7.94 \times 10^{14}$</td>
</tr>
<tr>
<td>SiC</td>
<td>1.50†</td>
<td>2.5</td>
<td>$2.08 \times 10^{15}$</td>
</tr>
</tbody>
</table>


† Energy for He interstitial surrounded by Si atoms – R. M. Van Ginhoven et al., 2006, J. Nucl. Mater., 51 348
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 $\nu_{\text{He}}^c$ value: $7.51 \times 10^{14}$

Gerasimenko, Mikhaĭlovskiĭ, Neklyudov, Parkhomenko, and Velikodnaya
3. Modelling: He embrittlement of GBs

Simple modelling of grain boundary (GB) failure

4. Critical bulk He concentration:

\[ G_{\text{He}}^c = \frac{3}{R} \nu_{\text{He}}^c \]

<table>
<thead>
<tr>
<th>Material</th>
<th>( \nu_{\text{He}}^c ) (cm(^{-2}))</th>
<th>( n ) (cm(^{-3}))</th>
<th>( G_{\text{He}}^c ) (appm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>( 6.90 \times 10^{14} )</td>
<td>( 8.5 \times 10^{22} )</td>
<td>488.0</td>
</tr>
<tr>
<td>Mo</td>
<td>( 8.05 \times 10^{14} )</td>
<td>( 6.4 \times 10^{22} )</td>
<td>753.2</td>
</tr>
<tr>
<td>Ta</td>
<td>( 7.77 \times 10^{14} )</td>
<td>( 5.5 \times 10^{22} )</td>
<td>841.3</td>
</tr>
<tr>
<td>W</td>
<td>( 9.16 \times 10^{14} )</td>
<td>( 6.3 \times 10^{22} )</td>
<td>871.5</td>
</tr>
<tr>
<td>Be</td>
<td>( 7.94 \times 10^{14} )</td>
<td>( 1.2 \times 10^{23} )</td>
<td>385.2</td>
</tr>
<tr>
<td>SiC</td>
<td>( 2.08 \times 10^{15} )</td>
<td>( 4.7 \times 10^{22} )</td>
<td>2645.6</td>
</tr>
</tbody>
</table>

- Assumed Grain size of \( R = 0.5 \mu m \)
- \( G_{\text{He}}^c \) varies linearly with \( 1/R \)
3. Critical lifetimes for GB embrittling by He

- Critical embrittlement lifetimes estimated using FISPACT

<table>
<thead>
<tr>
<th>Material</th>
<th>$G_{\text{He}}^c$ (appm)</th>
<th>Critical GB embrittlement lifetimes $t_{\text{He}}^c$ for DEMO</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Outboard FW</td>
</tr>
<tr>
<td>Fe</td>
<td>488.0</td>
<td>4 years</td>
</tr>
<tr>
<td>Mo</td>
<td>753.2</td>
<td>18 years</td>
</tr>
<tr>
<td>Ta</td>
<td>841.3</td>
<td>216 years</td>
</tr>
<tr>
<td>W</td>
<td>871.5</td>
<td>300+ years</td>
</tr>
<tr>
<td>Be</td>
<td>385.2</td>
<td>1 month</td>
</tr>
<tr>
<td>SiC*</td>
<td>2645.6</td>
<td>1.8 years</td>
</tr>
</tbody>
</table>

- 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)

Gilbert M R et al., 2012, *Nucl. Fus.*, 52 083019
Summary

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.