Evaluation of Tungsten as Divertor Plasma-Facing Material: Results from Ion-Irradiation Experiments & Computer Simulations

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8. UGC-DAE Consortium for Scientific Research, Indore, MP, India -452017
Tungsten as Plasma-Facing Material

- Low T-retention
- High melting point
- Low erosion

- Low dust formation
- Low $Z_{\text{eff}}$
- High heat flux handling

Neutron Irradiation & T-retention

What will be the T-retention in reactor environment?
Neutron flux & PKA spectrum for “ITER-like” reactor

Neutron transport calculations using ATTILA combined with SPECTER

PKA/neutron ~ 0.4

400 s shot
Even if only one D/T-atom was trapped at each defect ...

<table>
<thead>
<tr>
<th>Machine</th>
<th>Power (MW)</th>
<th>$\Gamma_n$ (cm$^{-2}$ s$^{-1}$)</th>
<th>FPY$^\S$ (lifetime)</th>
<th>$\Phi_n$ (cm$^{-2}$)</th>
<th>PKA$^\S$ (cm$^{-3}$)</th>
<th>FP$^{\S\S}$ (cm$^{-3}$)</th>
<th>T atom - trapped$&amp;&amp;$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ITER-like**</td>
<td>500</td>
<td>$1.7 \times 10^{13}$</td>
<td>0.4</td>
<td>$2 \times 10^{20}$</td>
<td>$8 \times 10^{19}$</td>
<td>$8 \times 10^{19}$</td>
<td>$4 \times 10^{25}$ (200 gm)</td>
</tr>
<tr>
<td>DEMO*</td>
<td>2000</td>
<td>$7 \times 10^{13}$</td>
<td>14</td>
<td>$3 \times 10^{22}$</td>
<td>$1.2 \times 10^{22}$</td>
<td>$1.2 \times 10^{22}$</td>
<td>$0.6 \times 10^{28}$ (30 kg!!!)</td>
</tr>
</tbody>
</table>

* DEMO based on ITER-like  
** Surface area $\sim$1000 m$^2$
$\S$ 1 FPY = $3 \times 10^7$ s
$\S$ PKA/n = 0.4
$^{\S\S}$ FP/PKA = 1
$\&\&$100 m^2 n$-wetted area (OVT+dome+IVT)

Assuming 20 years – 1.5kg/year  
Regulatory limit may force a de-tritiation/change

From the point of view of trapping it is crucial to understand the nature of defect and its relation to PKA
Number of defects & defect cluster size increases with PKA energy

Comparison with SRIM $E_d = 90$ eV. *Recombination is significant*

At lower PKA energies, ($E_{\text{PKA}} < 30$ keV) smaller defect clusters are formed.

![Graph showing the increase in number of defects with PKA energy with comparison to SRIM values.](image)

*Interstitials in red, Vacancies in green*

Atoms participating in the cascade $\sim 1/2$ ps have been superposed.

![Image showing defects at 20 keV and 20 ps after irradiation.](image)
As PKA energy increases larger interstitial & vacancy clusters are formed.
At even higher energies ($E_{\text{PKA}} > 150$ keV) splitting of cascades limit the cluster size.

215 keV: 2 separate cascades

375 keV: 1022 FP

PKA trajectory

Spatially & temporally interacting cascades

100 ps after bombardment

Vacancies leave the imprint of the cascade at room temperature
So far:

Correlation between PKA and defect needs to be studied for estimating T-trapping
Simulations show interstitials are mobile and show clustering at the end of the cascade
Vacancies are immobile at room temperature – leave the imprint of cascade

Ion-Irradiation Experiments

*Effect of PKA spectrum*
Parameters of irradiation experiments

<table>
<thead>
<tr>
<th>Ions (m) Energy</th>
<th>Mean Range (μm)</th>
<th>Fluence (cm²)</th>
<th>dpa E_d=90eV</th>
<th>Facility</th>
</tr>
</thead>
<tbody>
<tr>
<td>D⁺ (2) 100 keV</td>
<td>0.6</td>
<td>5 x 10^{17}</td>
<td>0.85</td>
<td>14 MeV n- generator, IPR</td>
</tr>
<tr>
<td>He⁺ (4) 250 keV</td>
<td>0.6</td>
<td>5 x 10^{15}</td>
<td>0.02</td>
<td>LEIBF, IUAC, Delhi</td>
</tr>
<tr>
<td>B³⁺ (11) 10 MeV</td>
<td>4.5</td>
<td>1.3 x 10^{14}</td>
<td>0.001, 0.01</td>
<td>3 MeV Tandem accelerator, Bilaspur</td>
</tr>
<tr>
<td>Au⁷⁺ (197) 80 MeV</td>
<td>4.5</td>
<td>1.3 x 10^{14}</td>
<td>0.22</td>
<td>15 MeV pelletron, IUAC, Delhi</td>
</tr>
</tbody>
</table>

Sequential irradiation of Au + D, B+D, He+D, Au+He+D
Recoil spectra for ions & neutrons

PKA of low mass ions are closer to neutrons

Is the defect structure similar?

Energy loss mechanisms, depth of penetration & heat
Recrystallized W-foil samples

- 0.8 x 0.8 x 0.1 mm$^3$
- 50 min at 1838 K in Ar+H

- Positron bulk-life time:
  \[
  \tau_1 = 107.3 \pm 1.7 \text{ ps (70%)}
  \]
  \[
  \tau_2 = 237.3 \pm 5.6 \text{ ps (30%)}
  \]

Multiple vacancies

Defect-free W: 105 ± 3 ps

Troev et.al., JPCS, 207 (2010) 012033

Annealing: S. Akkireddy et.al. EX/P4-12
Defect clusters – TEM studies
Defect cluster size of Au-irradiated samples is similar to neutrons.

Note: larger clusters in B-irradiation.

Cluster-size decreases with fluence.

*(Renterghem JNM 477 2016, p 80)*

*TEM Studies: P. Sharma et.al.  EX/P2-10*
The reason for cluster size difference is related to spacing between recoils.

Spacing between recoils within a cascade (>50 keV)

B ~ 10 nm
Au ~ 0.2 nm
Did others observe similar effects?
<table>
<thead>
<tr>
<th>S. No.</th>
<th>Author</th>
<th>Year</th>
<th>Journal</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>El-Atwani O. et al.</td>
<td>2015</td>
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<td>Hwang T. et al.</td>
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<td>Acta Materialia, 112, (105-120)</td>
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<td>21</td>
<td>Zhang Z. et al.</td>
<td>2015</td>
<td>J. Plasma Fusion Res. SERIES, 11</td>
</tr>
</tbody>
</table>
Heavy ion irradiation experiments show similar cluster size independent of energy and fluence

TRIM calculations were also carried out and found that heavy ions produce several PKA/particle close to each other over a *small depth range*. 
Competitive capture of mobile FP by seed clusters and dislocation lines?

Initial line density
$3.6 \times 10^8 \text{cm}^{-2}$

Mobile FP agglomerate and captured by fewer seeds large scale clusters & branching of lines

Shorter lines (80-1100 nm)
Higher density - $1.9 \times 10^{10} \text{cm}^{-2}$
Sparse clusters - $9.3 \times 10^9 \text{cm}^{-2}$

Long lines (400-3000 nm)
Lower density - $6.1 \times 10^8 \text{cm}^{-2}$
Dense clusters - $1.3 \times 10^{12} \text{cm}^{-2}$

Mobile FP – captured by several seeds small scale clusters and lines & Long lines
Irradiation with He (250 keV) & D (100 keV) ions
Cluster size of He irradiated samples is similar to Au-irradiation

250 keV He

5 x 10^{15} \text{ cm}^{-2} (0.02 \text{ dpa})

Line density 1.05 x 10^9 \text{ cm}^{-2}
Length 40 – 1000 nm

Cluster density 5.6 x 10^{10} \text{ cm}^{-2}
Size 5 – 15 nm

250 keV He

5 x 10^{17} \text{ cm}^{-2} (0.85 \text{ dpa})
Line density 9.7 x 10^8 \text{ cm}^{-2}
Length 120 – 1900 nm

Loops and network of dislocations clearly visible in D-irradiation

100 keV D
Clear loops

Diffusion & agglomeration of FP to form clusters

5 x 10^{17} \text{ cm}^{-2} (0.85 \text{ dpa})
Loop density 1.4 x 10^8 \text{ cm}^{-2}
Size 50 – 100 nm
So far:
Correlation between PKA and defect needs to be studied for estimating T-trapping
Simulations show interstitials are mobile and show clustering at the end of the cascade
Vacancies are immobile at room temperature – leave the imprint of cascade

*Interstitial cluster-size seem to depend only on the inter-PKA separation and hence on fluence*
*The capture of mobile FP by existing dislocation lines and existing clusters seem to explain the observed cluster sizes*
Positron life-time in the lattice  \( \tau = \frac{1}{\pi r_e^2 n_e c} \)
Multiple vacancy for Au, Single for B

The difference is good enough to distinguish between single & multiple vacancies

Fast $e^+$—$^{22}$Na source

$270$ keV

Penetration depth $\sim 16$ $\mu$m

Defect range $\sim 5$ $\mu$m

Defect-free W: $105 \pm 3$ ps

Troev et.al., JPCS, 207 (2010) 012033
Saturation indicates dense vacancy clusters in Au-irradiation

Slow $e^+$ beam - 0.1 to 30 keV
Doppler broadening of 511 keV $\gamma$
$S - e^+-e^-$ from valance electrons
$W - e^+-e^-$ from core electrons

similar effects: $20 \text{ MeV} W$, MF Barthe et al.\textsuperscript{26}
He & Au shows saturation of S-parameter, indicating saturation of vacancies in the $e^+$ penetration range.

Similar observations: P.E. Lhuiller et.al, JNM 433 (2013), Troev et.al.,NIMB 267 (2009)
Deuterium creates defects within 400 nm and D atoms are trapped in these defects(?)

No saturation is seen unlike Helium

Change in slope indicates annihilation from different core electrons than W
Most of the deuterium found to be less than 500 nm

7.3 MeV C\(^{6+}\)

15 keV Cs\(^+\) ions; 23° to normal

1 s = 0.5 nm
Deuterium depth profile in pre-irradiated tungsten

B-irradiated sample seem to trap more D than Au-irradiated sample.

Single vacancy traps more D than multiple vacancies (*Ahlgren et.al, JNM 2012*)

It seems from PAS that B-irradiation creates more single vacancies as opposed to Au.

*Ongoing investigations*
So far:
Correlation between PKA and defect needs to be studied for estimating T-trapping
Simulations show interstitials are mobile and show clustering at the end of the cascade
Vacancies are immobile at room temperature – leave the imprint of cascade

Interstitial clustering seem to depend only on the inter-PKA separation and hence fluence
The capture of mobile FP by existing dislocation lines and existing clusters seem to explain
the observed cluster sizes

Vacancy show the imprint of cascade and hence related to the PKA energy and their spectrum
T-trapping takes place predominantly at vacancies
Conclusions & Outlook

Correlation between PKA and defect needs to be studied for estimating T-trapping
Simulations show interstitials are mobile and show clustering at the end of the cascade
Vacancies are immobile at room temperature – leave the imprint of cascade

Interstitial clustering seem to depend only on the inter-PKA separation and hence on fluence
The capture of mobile FP by existing dislocation lines and existing clusters seem to explain the observed cluster sizes

Vacancies show the imprint of cascade and hence related to the PKA energy and their spectrum
T-trapping takes place predominantly at vacancies

Accurate quantification of T-retention requires precise estimation of vacancies – using a combination of surrogate ions with controlled fluence of different mass, energy and temperature is urgently needed.
Overall Programme

D-retention

Goal 1: Estimation of D-Retention in W, in presence of He & Alloying elements

E1, E2 = 2 deuterium energy (80keV, 100keV)
D1, D2, D3 = Damage energy
D1F1, D1F2, D1F3 = Damage fluence

D-Retention

Multi-Scale Modelling

Damage

Goal 2: Damage studies, defect and microstructure of irradiated W & alloys

Thank you!
Backup slides
In a given cascade

Crowdions have the highest mobility and formation energy.

Mobility of interstitial clusters are limited.
The reason for difference lies in the PKA spectra.

Spacing between recoils within a cascade (>50 keV)

5000 trials

B ~ 10 nm
Au ~ 0.2 nm
Larger Sparse Loops in B-Irradiation

- Line density - $1.9 \times 10^{10}$ cm$^{-2}$
- Line length – 80 – 1100 nm
- Cluster density - $9.3 \times 10^9$ cm$^{-2}$
- Loop density – $6.9 \times 10^8$ cm$^{-2}$
Depth Profile of Point Defects

- Saturation of S - Au irradiation

  similar effects: 20 MeV W, MF Barthe et al

- Fewer defects in Boron

- Vacancy clusters/loops
Au & N-irradiation Produce Small Clusters

Similar defect size distribution for heavy ions at 300 K and neutrons at 1000 K

At high temperature heavy ions produce clusters similar to 300 K boron irradiation