Retention behavior of H isotopes in W revisited by multi-scale modelling

Presented by Jie Hou

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Outline

- Backgrounds
- Methodology
- Results
- Conclusion
Backgrounds

W is the most promising PFM

Fuel loss
- JET: Over 30% (11.5g/35g, 1997), mainly retained in PFM
- CFETR: TBR=1.2, needs to <~1%

PFM failure
- High fluence (>~ $10^{23} H/m^2$) implantation cause surface blistering and peeling

Interaction with H(D/T) limits its uses
Backgrounds

**Thermal Desorption Spectra:**

- Temperature
- Ion energy
- Fluence
- TDS
- Composition
- Micro-structure

**Fundamentals of H retention are not fully understood**

Ogorodnikova. 2003

Wang, P. 2015

Images showing thermal desorption spectra with varying temperature and fluence conditions.
Methodology

Electronic calculation (VASP) + Large scale simulation (OKMC) = Experiments

Ion implantation database (IM3D) + Input = Interpret

Verify
Results: Vacancy binding energies

1. H trapped at the inner wall rather than the center of small V clusters.
2. Binding energy decreases linearly with trapped H atoms.
3. H capacity is proportional to surface area of V clusters.
Results: Impurity binding energies

Our previous study of H binding to O, C and transition metal impurities.

X.-S. Kong 2013

X.-S. Kong 2016
Results: Kinetic barriers

1. $E^V_{m} = 1.65 \text{ eV}$, become mobile at $\sim 550 \text{ K}$

2. $E^H_{m} = 0.25 \text{ eV}$, become mobile at $\sim 80 \text{ K}$

3. $E^{V_1-H_1}_{t} = 1.44 \text{ eV}$, detraps at $\sim 480 \text{ K}$
Results: H retention in damage free W

Effect of dilute impurities on H trapping:

<table>
<thead>
<tr>
<th>Exp. Ref.</th>
<th>$E_{ion}$ (keV)</th>
<th>$F$ ($H/m^2$)</th>
<th>$f(H/m^2/s)$</th>
<th>T (K)</th>
<th>$C_{imp}$ (appm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soltan. 1991</td>
<td>0.2</td>
<td>$1.8\sim2.6 \times 10^{16}$</td>
<td>$1\sim4 \times 10^{15}$</td>
<td>5</td>
<td>10-100</td>
</tr>
</tbody>
</table>

1. ~80 K: Activation of H migration.

2. ~160 K: De-trapping from 100 appm oxygen impurity.

3. ~450 K: De-trapping from 5 appm V.

![Graph showing H retention and trapping effects](image)
Results: H retention in damaged W

Effect of irradiation damages on H trapping:

<table>
<thead>
<tr>
<th>Exp. Ref.</th>
<th>$E_{ion}$ (keV)</th>
<th>F ($H/m^2$)</th>
<th>f($H/m^2/s$)</th>
<th>T (K)</th>
<th>$C_{imp}$ (appm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ogorodnikova. 2008</td>
<td>0.2, 3</td>
<td>$1 \times 10^{22}$</td>
<td>$2.5 \sim 9 \times 10^{19}$</td>
<td>300, 380</td>
<td>100</td>
</tr>
</tbody>
</table>

1. H trapped mainly by impurities in undamaged W.

2. H retention is greatly enhanced by irradiation damage.

3. H trapping is dominated by V1 and small V clusters.
Results: H retention in damaged W

Depth profile:


2. Bulk region: H retention dominated by impurity atoms.

Depth profile after 3 keV D implantation, embedded figure shows details of the first 100 nm.
Results: H retention in damaged W

Saturation nature:

1. $F < \sim 10^{20}$: ~100% retention due to abundant V.

2. $\sim 10^{20} < F < \sim 3 \times 10^{21}$: All V filled up with H, retention limited by V survival rate.

3. $F > \sim 5 \times 10^{21}$: V saturated due to high V-I recombination rate, so does the H retention.
Conclusion

- DFT-based multi-scale model is implemented to understand H retention mechanism.

- Even very dilute impurities can influence H retention significantly due to its wide distribution.

- Ion irradiation damage concentrates at near-surface region. It increases H retention greatly, but saturates at high fluences.
Thank you