Migration of rhenium and osmium in tungsten

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Neutron irradiation to W causes Re and Os through nuclear transmutation

Principal transmutation path for W

\[
\begin{align*}
^{186}W(n, \gamma)^{187}W \\
\rightarrow (\beta^{-})^{187}Re
\end{align*}
\]

\[
\begin{align*}
(n, \gamma)^{188m}Re \rightarrow (\gamma)^{188}Re \rightarrow (\beta)^{188}Os \\
(n, 2n)^{186}Re \rightarrow (\beta^{-})^{186}Os
\end{align*}
\]

\[
^{184}W(n, \gamma)^{185}W \rightarrow (\beta^{-})^{185}Re(n, \gamma)^{186}Re \rightarrow (\beta^{-})^{186}Os
\]

at the first wall

Pure W → W-18Re-3Os* (50dpa)

W-6Re-3Os** (end-of-service)


Microstructure evolution of W-Re under neutron radiation environment*

*Hasegawa et al., Fusion Engineering and Design, 89 (2014) 1568–1572

Void lattice may collapse, and RIP takes place?

Establishing a quantitative model is essential.
RIP development mechanism


Detailed mechanism of ③ is not known.
Solute migration is essential for RIP

Solid solution in thermodynamic equilibrium

- Defect energy
- Cascade displacement or Frenkel pairs
- Radiation

Solute migration & V-I recombination

- Solute migration
- V-I recombination

Precipitated (σ-phase or χ-phase)

Phase transformation

- Annealing?
- Solutes become aggregated.

Present study aimed to investigate mobility of Re&Os in W.
Modeling Method

- Density functional theory (DFT)
- **VASP** (Vienna ab initio Software Package)
- Projected augmented wave potential (PAW/PBE)
- 4$a_0$ × 4$a_0$ × 4$a_0$ (128 atoms) super cell
- K-point (3 × 3 × 3)
- Cutoff energy: 350eV
- Volume relaxation

128-lattice super cell
Results
Solute atom and point defects are all attractive.

\[ E_{b}^{\text{sol},\alpha} = E_{f}^{\text{sol}} + E_{f}^{\alpha} - E_{f}^{\text{sol},\alpha} \]

\( \alpha \): vacancy or SIA

\( E_{\text{sol, vacancy}} \): Vacancy is located at 1\textsuperscript{st} and 2\textsuperscript{nd} NN position of solute atom;

\( E_{\text{sol, SIA}} \): The most stable mixed-dumbbell configuration.

<table>
<thead>
<tr>
<th></th>
<th>1NN Vacancy (eV)</th>
<th>2NN Vacancy (eV)</th>
<th>SIA (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Re</td>
<td>0.22</td>
<td>0.22</td>
<td>0.79</td>
</tr>
<tr>
<td>Os</td>
<td>0.53</td>
<td>0.36</td>
<td>1.87</td>
</tr>
</tbody>
</table>

Condition for RIP development

① SIA and solute atom is attractive.
② Vacancy and solute atom is attractive.
③ Solute atoms must be dragged by SIA or vacancy.
Interstitional mode of solute migration is dominant.

Point defect migration energy in W-Re and W-Os alloys (Evaluated by nudged elastic band method)

<table>
<thead>
<tr>
<th></th>
<th>Vacancy Mode</th>
<th>Interstitial Mode*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Re</td>
<td>1.65</td>
<td>0.12</td>
</tr>
<tr>
<td>Os</td>
<td>1.43</td>
<td>0.27</td>
</tr>
<tr>
<td>Self (W)</td>
<td>1.69</td>
<td>0.01</td>
</tr>
</tbody>
</table>

* Migration between most favorable mixed dumbbells

Interstitial mode of Re (Os) migration is focused.
SIA has 1-dimensional motion

SIA formation energy

Self-Interstitial Atom (KMC)
$<111>$ W-Re mixed dumbbell has 3D motion

Re-interstitial formation energy

Rotation barrier is low.
Low rotation barrier enable Re to migrate.

KMC for imaginary mixed dumbbell with rotation barrier as high as SIA

Low rotation barrier is essential to Re migration (i.e. RIP).
<110> W-Os mixed dumbbell has 3D motion
Discussion: Does 3D motion suppress radiation swelling?

KMC for cascade annealing

Surviving SIA ratio

Defects with 3D motion promotes V–I recombination
Summary

- Re and Os in W, which are generated by transmutation, satisfy the three essential conditions for RIP.
- Re- and Os-interstitials become stable mixed dumbbell and has 3D migration mode.
- Stabilization of <110> mixed dumbbell:
  1) causes solute migration, i.e., RIP?
  2) promotes V–I recombination and suppress swelling?

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