Molecular dynamics simulations of the clustering and dislocation loop punching behaviors of noble gas atoms in tungsten


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Tungsten: one of the most promising candidate PFM.

- high melting point
- high thermal conductivity
- high physical sputtering threshold energy
- Low sputtering rate
- Low fuel (deuterium/tritium) retention ...

**ASDEX Upgrade**: A full tungsten divertor for ITER has passed the test

**EAST**: Recently, the PFM changed from total C to C and from W to total W.

**ITER**: The PFM changed from Be/C/W to Be/W and then from W to total W.

PFMs changed from other materials to W gradually during the upgrade process of tokamak.
the formation of fuzzy structures on tungsten caused by helium plasma irradiation

The low energy and high-flux He plasma irradiation

Before

After

SEM

(a)~(c): SEM photographs of W-C surface after and before helium plasma irradiation at a surface temperature of 1250K, a fluence of $3.5 \times 10^{27}\text{m}^{-2}$ and an ion incident energy of 12eV. (d) and (e): photographs taken by FE-SEM with a high spatial resolution. The line of sight is normal to the samples.

The problems existing in the study of Fuzz on W surface

The physical mechanism of the formation of Fuzz are not entirely clear up to now.

- Helium bubble nucleation, growth and rupture play a key role in formation of Fuzz.
The problems existing in the study of Fuzz on W surface

As noble gas plasma, why the Fuzz not form by Ne or Ar plasma irradiation?

1. The diffusion, trapping and clustering properties of the three noble gas atoms are different;
2. The rupture process of three noble gas bubbles in the near surface in W is different;
3. The different penetration depth of three noble gas atoms lead to the different microstructure evolution;

Even under the irradiation condition under which tungsten nanostructures can be formed by He plasma irradiation, holes/bubbles and fiber-form nanostructures were not formed on the surface by exposing to Ar or Ne plasmas.

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To explore the mechanism behind the phenomenon, the behaviors of noble gas X (=He, Ne and Ar) atoms

a) in the bulk of W

b) on the surface of W

have been studied with molecular dynamics simulations. The adopted code is MOLDY.
The interatomic potentials
The interatomic potentials

The potentials between atoms is the basis of molecular dynamics simulation.

Potentials we choose are as follows:

The interactions between same atoms:

W–W:


He–He, Ne–Ne, Ar–Ar:


The interactions between different atoms:

W–He, W–Ne, W–Ar:

The EAM potential of W–W


Interatomic potentials for modelling radiation defects and dislocations in tungsten

\[ E (r_1, \ldots, r_N) = \sum_{i=1}^{N} \left[ \sum_{j>i}^{N} \Phi(r_{ij}) + F(\rho_i) \right], \]

\[ \Phi (x) = \sum_{i=1}^{n^\Phi} a_i^\Phi (\delta_i^\Phi - x)^3 \Theta (\delta_i^\Phi - x), \]

\[ \rho (x) = \sum_{i=1}^{n^\rho} a_i^\rho (\delta_i^\rho - x)^3 \Theta (\delta_i^\rho - x), \]

\[ F (x) = a_1^F \sqrt{x} + a_2^F x^2. \]

\[ \Theta(x) : \text{Heaviside step function} \]
The potentials of He–He, Ne–Ne and Ar–Ar

**HFD–B** (Hartree-Fock-dispersion) form

\[ U(r) = \varepsilon \, V^*(x) , \]

\[ V^*(x) = A^* \, \exp(-\alpha^* x + \beta^* x^2) - \left(\frac{C_6}{x^6} + \frac{C_8}{x^8} + \frac{C_{10}}{x^{10}}\right)F(x) , \]

\[ F(x) = \begin{cases} 
\exp[-\left(\frac{D}{x} - 1\right)^2], & x < D, \\
1, & x \geq D, 
\end{cases} \]

where \( x = r / r_m \).

\( \varepsilon, A^*, \alpha^*, \beta^*, C_6, C_8, C_{10}, D \) and \( r_m \) are constants.

The potential of W–X (He, Ne, Ar) :

\[ U = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} V(r_{ij}) + \sum_{i=1}^{N} F_s(\rho_s^i) \]

Pair potential  Many body interaction

\[ V(r) = \sum_{k=1}^{9} a_k (r_k - r)^3 \times H(r_k - r) \]

\( H(r_k - r) \): Heaviside function
The potential of W–X: many body interaction

S-Band for W-X:

\[ F_s (\rho_s) = b_1 \sqrt{\rho_s} + b_2 \rho_s^2 \]

1s-type and 6s-type Slater functions for He and W:

\[ \chi^{1s} = N_{1s} \exp(-\xi_{1s} r) \]
\[ \chi^{6s} = N_{6s} r^5 \exp(-\xi_{6s} r) \]

total function:

\[ \phi_s^{W-He} = N_s r^5 \exp(-2\xi_s r) \]
\[ \xi_s \] is an average from the 1s and 6s Hartree-Fock orbitals for He(\(\xi_{1s}\)) and W (\(\xi_{6s}\)).

The potential of W–X: many body interaction

\[ \phi_s^{W-Ne} = N_s r^6 \exp(-2\xi_s r) \]

\[ \phi_s^{W-Ar} = N_s r^7 \exp(-2\xi_s r) \]

Ns is chosen to be 20.0. \( \xi_s \) is an average \( \xi \) (Slater orbital exponent) from the 1s/2s/3s and 6s Hartree-Fock orbitals for He/Ne/Ar and W, respectively.

Total electron density of an atom calculated from \( s \)-band model

\[ \rho_s = \sum \phi_s^{FeHe} \]

Physical meaning of the electron density!

Initial simulation model
The simulation of nucleation of noble gas in W

Initial model:
Blue balls are noble gas atoms (He/Ne/Ar)
Background atoms (W) are invisible

The system size: $45a_0 \times 45a_0 \times 45a_0$, $a_0$ is the lattice constant
The number of W atoms: 182250
The number of X atoms: 125 (evenly distributed, the concentration is 685 appm)
Temperatures: 400K, 1200K, 2000K
The simulation of dislocation loop punching

periodic boundary conditions were applied in X and Y directions

The box size: \(20a_0 \times 20a_0 \times 50a_0\)

Temperature: 1200K

The depth of He/Ne/Ar cluster: \(4x a_0 \sim 7x a_0\)

crystal orientation of Z axis: \(<100>\ <110>\ <111>\)

Noble gas atom is added one by one
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The initial nucleation of He/Ne/Ar clusters

Related factors:
- diffusivity
- dissociation/absorption
The diffusion of X atom and small clusters in W

![Graphs showing lnD vs. 10^3/T for different species](image)

- **Temperature range:** 500-1400K

\[
MSD = \langle [r_i(t) - r_i(0)]^2 \rangle
\]

\[
D = \frac{MSD}{6t}, \quad D = D_0 \exp\left[-\frac{E_m}{k_B T}\right]
\]

\( E_m \) is proportional to the slope.
When the gas cluster becomes larger, SIA emission can happen. It is much more difficult for noble gas cluster, combined with SIA-V(cluster), to diffuse in tungsten.
Noble gas cluster induced SIA emission

Minimum temperature for He/Ne/Ar cluster to emit SIA(cluster)

SIA emission can happen at low temperature when the size of He reaches 6, and for Ne/Ar the corresponding size is as small as 2.
dissociation of small noble gas cluster in W

Simulation temperature: < 2000K
Cluster size minimum dissociation temperature
2 He atoms 1400K
3 He atoms 1600K
4 He atoms 1800K

It is rare to see dissociation process while size of He cluster larger than 4, as for Ne and Ar, it is hard to see that even in size of two
The binding energies between X and X clusters

(a) A X atom binding to X_n cluster

(b) A X (He, Ne and Ar) atom binding to X_n-V cluster

\[ E_b(X) = E_f(X) + E_f(X_nV_m) - E_f(X_{n+1}V) \]

◆ Biding energies: Ne, Ar > He
Clustering of He in W (3D snapshot)

He clusters in W bulk, simulation

time 2.0 ns at 1200K

Separated clusters are colored differently

Max cluster size: 7 atoms
Clustering of Ne in W

Ne clusters in W bulk, simulation
time 2.0 ns at 1200K
Separated clusters are colored differently
Max cluster size : 4
Clustering of Ar in W

Ar clusters in W bulk, simulation

time 2.0 ns at 1200K

Separated clusters are colored differently

Max cluster size : 5
At 400K, He clusters is small due to its low mobility at low temperature. Most of gas atoms are dissociative. At higher temperature, clusters grows larger as temperature increasing. Then SIAs are emitted. At 2000K, dissociative atoms are still the main part of He due to frequent dissociation activities.
Clustering of Ne in W

Ne cluster size distribution at different temperature
Simulation time 1.6 ns

SIA cluster size distribution at different temperature
Simulation time 1.6 ns

No clusters are observed at 400K.
At higher temperature, lots of SIAs are emitted, the largest size of SIA cluster is up to 21 atoms.
Clustering process is accelerated when temperature rises.
Clustering of noble gas in W

Ar cluster size distribution at different temperature
Simulation time 1.6 ns

SIA cluster size distribution at different temperature
Simulation time 1.6 ns

No remarkable differences from Ne
Comparison between He, Ne and Ar at 1200K

Max size of Ne or Ar cluster is smaller than He.
SIAs emitted by He cluster is less than Ne/Ar
The simulation of dislocation loop punching
Tungsten surface evolution by helium bubble nucleation, growth and rupture

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Dislocation loop punching——The origin of Fuzz on W surface?
Figure 4. Evolution in time of the helium bubble, tungsten interstitials, and surface adatoms during growth of a helium bubble below a tungsten (1 0 0) surface (a)–(g). Trap-mutation processes of single interstitial formation repeatedly occur as gas pressure increases, leading to the self-assembly of prismatic loops, which de-trap from the bubble and glide to the surface, forming multiple adatom ‘islands.’ Ultimately, the bubble ruptures (g), (h), leaving a heavily deformed surface (i) with multiple layers of tungsten adatom ‘islands,’ a crater, and a hole. Red spheres are vacant sites, green are displaced tungsten atoms, purple are surface adatoms, blue spheres are helium, and grey spheres are tungsten atoms. Images made with AtomEye [36].
The simulation of dislocation loop punching

- Periodic boundary conditions were applied in X and Y directions.
- Box size: $20a_0 \times 20a_0 \times 50a_0$.
- Temperature: 1200K.
- Depth of He/Ne/Ar cluster: 22.16~12.66Å.
- Crystal orientation of Z axis: <100> <110> <111>.

Noble gas atom is added one by one.
Loop punching in the near surface of W
Loop punching in the near surface of W

Ne
Depth: 7x\(a_0\)
Video made with OVITO
Loop punching in the near surface of W

He
Depth: 7\times a_0
# Loop punching in the near surface of W

Cluster depth: $4Xa_0$ ($a_0$ is the lattice constant)

<table>
<thead>
<tr>
<th></th>
<th>He</th>
<th>Ne</th>
<th>Ar</th>
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<tr>
<td>100</td>
<td>27/57</td>
<td>40/60</td>
<td>13/16</td>
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<tr>
<td>110</td>
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<tr>
<td>111</td>
<td>14/48</td>
<td>24/45</td>
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Cluster depth: $5Xa_0$

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<tr>
<td>111</td>
<td>15/77</td>
<td>15/63</td>
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Cluster depth: $6Xa_0$

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<tr>
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Cluster depth: $7Xa_0$

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<th>Ar</th>
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<td>39/153</td>
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<td>76/296</td>
<td>33/202</td>
<td>77/</td>
</tr>
<tr>
<td>111</td>
<td>75/343</td>
<td>38/248</td>
<td>22/133</td>
</tr>
</tbody>
</table>

**Demonstration: A/B**

**A:** cluster size when loop punching for the first time  
**B:** cluster size when bubble burst
Loop punching in the near surface of W

The difficulty of loop punching is approximately follow rules

Type of noble gas: He > Ne > Ar
Surface orientation 100 > 110 > 111

The simulations show that when the noble gas cluster is large enough, loop punching will happen. The bubble will burst after a couple of times of loop punching, forming adatom island on the surface of W.
There is no big different between He/Ne/Ar.
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Conclusion

Based on the empirical W-X potentials developed recently in our group, the formation of clusters and bubbles of the three noble gases in W bulk was simulated at the temperatures from 400K to 2000K.

Results show that higher temperature promotes the nucleation of X bubbles, and the SIAs and X-vacancy clusters for Ne and Ar are much larger than those of He, which indicates that Ne and Ar atoms can be trapped more easily by SIA clusters.

The behaviors of noble gas X (=He, Ne and Ar) atoms on the surface of W have been studied with molecular dynamics simulations. When the sizes of the X bubbles are large enough in W, the behavior of dislocation loop punching is observed for all the three noble gas.
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