P30A

# Molecular Dynamics Simulations of Atomic Carbon on Tungsten Surface

Zhongshi Yang[a,b], Qian Xu[a], Rongjie Hong[a], Guang-Nan Luo[a]

[a]*Institute of Plasma Physics, Chinese Academy of Sciences, Hefei, China*
[b]*Max-Planck-Institut für Plasmaphysik*, Garching, Germany

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## Motivation

- **Tungsten (W) as candidate PFM** for EAST, ITER and future DEMO reactors
- **The inevitable mixing of C with W** in the scenario where the PFM is made from a combination of C and W in fusion devices
- **Interaction between low energy C and W** surface for C particles in divertor region are reduced below 100 eV
- **Necessity** to understand and predict the W surface properties and performance in the presence of C impurities
- **Molecular dynamics (MD)** for accurate simulation in the low energy range: scarce experimental data, BCA model breaks down, many-body nature

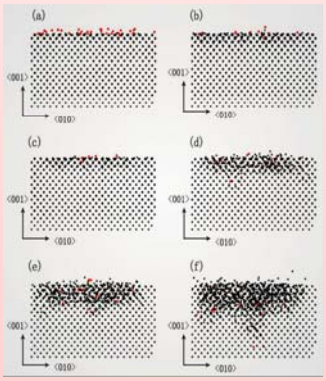
## Simulation Methods

- **Initial BCC W cells**: variable dimensions according to the incident C energies, consisting of 2000～10000 atoms, density of 19.25 g/cm$^3$
- **Surface creation:** periodic boundary conditions removed in the z direction, the atoms in the lowest three atomic layers kept fixed at their original positions all times
- **C bombardments**: an C atom placed at a fixed distance from the surface assigned a velocity toward the surface with kinetic energies ranging from 0.01 eV to 200 eV
- **Simulation termination**: (i) backscattered atoms with a distance from the surface greater than the potential cut-off distance, (ii) absorbed atoms with kinetic energy lower than C migration energy
- **Potential**: Analytical bond-order interatomic potential for modeling nonequilibrium processes in the W–C system *

** N. Juslin, et al., J. Appl. Phys. 98 (2005) 123520*

## Results and Discussion

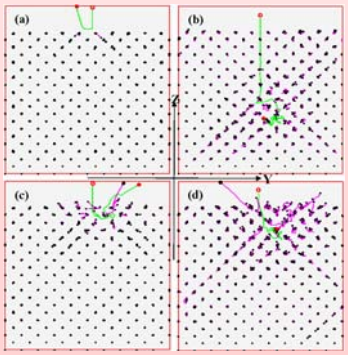
### Cumulative Irradiation




***Snapshots of the simulation cells*** *after successive 50 incident energetic projectiles' bombardment at (a) 1 eV (b) 5 eV (c) 10 eV (d) 50 eV (e) 100 eV (f)200 eV*
**red balls represent the C atoms*
**black ones represent W atoms*

- The amorphization is pronounced with increasing $E_i$
- The kinetic energy of the projectiles is released through fast collisions with contiguous lattice atoms, while temperature in the impact area and vibration amplitude of lattice atoms increase

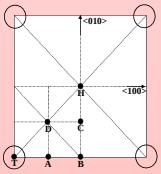
### Surface Sputtering




***Four types of energy deposition processes*** *for energetic C atom with $E_i$=150 eV on W surface: (a) direct reflection, (b) channeling, (c) delayed reflection (d) trap near top surface*

- Surface sputtering is related to the energy deposition processes

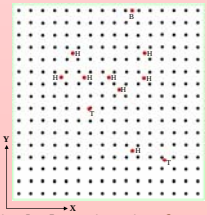
### Adsorption of C on W




**Adsorption sites on W top surface**

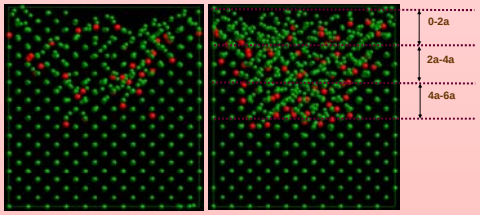
***Formation energy of different sites of C on W (100) surface***

| Site | H | C | B | A | D | T |
|---|---|---|---|---|---|---|
| $E_f$ (eV) | 1.013 | 1.912 | 1.725 | 2.555 | 1.357 | 3.285 |

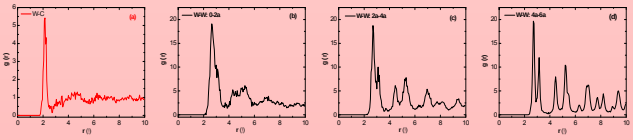



***Final adsorption sites for C atoms*** *on W (001) surface with $E_i$=0.1eV,* ***11 C atoms of all 30 incident projectiles*** *are stuck on surface (H: hollow site, T: top site)*

### C-W Mixed Layers



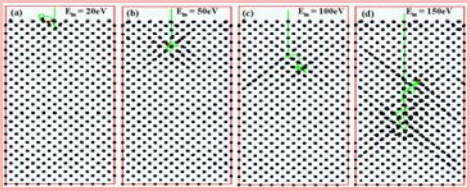

***C-W mixed layers:*** *(a) 100 C atoms projected on the W surface; (b) 200 C atoms projected on the W surface*




*W-C pair distribution function g(r) (a)* and *W-W pair distribution function g(r) at different depth from the surface: (b) 0 -2a, (c) 2a - 4a, (d) 4a – 6a, a is lattice constant of bcc-W*

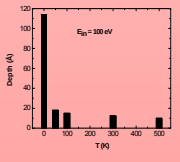
- 0 - 2a, typical amorphous structure from g(r) for W-W
- > 4a, near to crystalline structure from g(r) for W-W

### Channeling

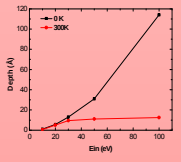



- 20 eV, L=a
- 50 eV, L=2a
- 100 eV, L=4a
- 150 eV, L=12a

***Trajectories of channeled*** *C atoms in W lattice with different $E_i$: (a) 20 eV; (b) 50 eV; (c) 100 eV; (d) 150 eV*




***Channeled depth*** *with different substrate temperature at $E_i$ 100eV*




***Channeled depth*** *with different $E_i$ at $T_{sub}$=0K and $T_{sub}$=300 K separately*

- Channeled depth is sensitive to the substrate temperature
- Channeled depth increases dramatically with $E_i$ at $T_{sub}$=0 K

## Conclusions

- MD simulations was performed to study the interactions between C and W using a bond-order interatomic potential
- Surface sputtering is related to the energy deposition processes
- At low $E_i$ ,C is apt to stick on the hollow site of the surface
- At high $E_i$, channeling effects occur varying with surface temperature
- C-W mixed layer showing typical amorphous structure