Effect of thermal and collisional processes on the performance of plasma-facing components in mixed materials environment

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Models and Data for Plasma-Material Interaction in Fusion Devices
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Outline

- ITMC-DYN package - self-consistent analysis of collisional and thermal processes
- Nanolayers build-up and mixing
- Chemical compounds on D recycling from Li surfaces
- Effect of thermal processes on C implantation and W erosion
- Mixed C/D ion beams on W erosion
Models Development and Benchmarking at Purdue University

High Energy Interaction with General Heterogeneous Target Systems (HEIGHTS)

IMPACT lab

Center for Materials Under Extreme Environment (CMUXE)
HEIGHTS Dynamic Simulation of Particle Beam Mixing with Target Materials—ITMC-DYN Code

Ion Transport in Materials and Compounds

ITMC Code

Fully 3D multi-beam on multi-target/layer compositions

ITMC-DYN: multi-component, surface evolution

T. Sizyuk and A. Hassanein, J. Nucl. Mater. 404, 2010 60
- Collision models are integrated with detail models of time-dependent processes including atom diffusion and segregation.
- Moving boundary conditions for sputtering erosion or surface growth.
Benchmarking of Dynamic Update of Materials Composition

- Nano-scale multilayers formation – 90 eV Fe\(^+\) and 50 eV C\(^+\) -> Si

![High-resolution TEM micrograph of Fe/C multilayers with 4 bilayer periods: ~0.75 nm, ~1.25 nm, ~2.5 nm and ~5.0 nm in order from the Si substrate, respectively.](image)

- ITMC-Dyn – 4 bilayer periods: ~1.1 nm, ~1.8 nm, ~2 nm, ~4.3 nm. (each from 2 bilayers)
ITMC-DYN: Simulation of Ions interaction with Multi-Layer Mirrors (EUV Lithography)

MLM surface response to Sn ions with low energy – around 50 eV

MLM surface response to Sn ions with high energy – around 2.5 keV

http://www.nist.gov/pml/div685/extreme-uv-lithography.cfm/

Response of MLM Layers to 1 keV Gd Ions Irradiation
(future beyond EUV Lithography)

More mixing and damage of MLM with La layers – due to lower density and lower surface binding energy of La

Modeling of D interaction with Li and compounds

- Three important processes for hydrogen interaction with liquid lithium surfaces – reflection, diffusion, and surface recombination.

Using experimental results for hydrogen isotopes diffusion in Li and compounds, we estimated/calculated the diffusion coefficient in multi-component materials depending on target composition as the interpolation of logarithmic values of diffusivity in each compound.

R.E. Buxbaum, et al., 24 (1985) 180
Surface Composition and Deuterium Recycling – starting from pure Li

10^{22} \text{ m}^{-2}\text{s}^{-1} 1 \text{ keV deuterium flux}
3\% 3 \text{ keV carbon ions}
0.1\% 3 \text{ keV oxygen ions}

Deuterium reflection and diffusion in Mo with thin (~10 nm) Li coating

Variation in initial Li compound thickness from 100 nm to 200 nm results in four times difference in deuterium desorption

Variation in carbon ions concentration in edge plasma from 1% to 3% results in two times difference in deuterium desorption.

Mixed Ions Beam on W erosion and C Implantation

Ion beams consisted of 70% of 333 eV H\(^+\), 10% of 500 eV H\(^+\), 20% of 1 keV H\(^+\), and C ions with 1 keV energy.

Concentration of C in tungsten at temperature 653 K for various C concentrations in ion beam


Mixed Ions Beam on W erosion and C Implantation

Hydrogen with impurities on reactor walls

H & C ions $\rightarrow$ W at 1000 K

Carbon accumulation, sputtering and diffusion


Carbon accumulation, sputtering and diffusion + Surface segregation after irradiation

Modeling of Surface Segregation

\[ \frac{\partial C_s(t)}{\partial t} = \frac{M}{a_1^2} C_1(t) \left[ \Delta G + kT \ln \frac{C_1(t)(1-C_s(t))}{C_s(t)(1-C_1(t))} \right] \]

\[ \frac{\partial C_i(t)}{\partial t} = M kT \left[ \frac{C_{i+1}(t)}{a_{i+1}^2} \ln \frac{C_{i+1}(t)(1-C_i(t))}{C_i(t)(1-C_{i+1}(t))} - \frac{C_i(t)}{a_i^2} \ln \frac{C_i(t)(1-C_{i-1}(t))}{C_{i-1}(t)(1-C_i(t))} \right] \]

$C_s$ and $C_i$ – the relative concentrations at the top surface and at the $i^{th}$ layer of the bulk; $a_i$ – the thickness of $i^{th}$ layer; $\Delta G$ - the segregation energy; $M$ - the mobility parameter

\[ D = M kT \left( 1 + \frac{\partial \ln f}{\partial \ln C} \right) \]

$D$ – the diffusion coefficient

$f$ - the activity coefficient of alloy components

In ideal or dilute solution: \[ M = \frac{D}{kT} \]

Target Temperature on W erosion and C implantation - Experiments

W sputtering by C ions at different target temperatures


Surface Segregation and Diffusion at Elevated Temperatures

Carbon implantation at 300 K and 870 K. Ion beam: $10^{18}$ m$^{-2}$s$^{-1}$, 6 keV at $15^\circ$ (to normal)


ITMC-DYN modeling - will be published
Relation between the diffusion coefficient (Fick’s model) and the mobility parameter for the bulk (Darken modified by de Plessis) ($\Delta G = 2$ eV; $M_s = 10^{-21}$ m$^2$s$^{-1}$/kT)

ITMC-DYN modeling - will be published
Surface Segregation and Diffusion at Elevated Temperatures

Carbon layer build-up at 300 K

Enhanced W erosion at 870 K

ITMC-DYN modeling - will be published
Surface Composition on Carbon Implantation

0.6 sputtering and reflection yield

0.85 sputtering and reflection yield

Only diffusion in modeling - 0.65 sputtering and reflection yield
Ions Flux and Composition Dependence

Dependence of tungsten erosion on C ion flux at 870 K

Dependence of W erosion / C implantation on C content in beam with D ions at 870 K


ITMC-DYN modeling - will be published
Ions Beam Energy and Composition + Thermal Effects on Tungsten Erosion

Composition at steady-state
Effect of D ions energy on W erosion and C implantation
**Summary**

- Recent upgrade and development of ITMC-DYN package explained several recent and interesting experimental results.

- Minute impurity contents in plasma can significantly affect erosion lifetime, cause significant increase hydrogen isotope retention, and enhance bubble/blister formation in candidate reactor materials in fusion environments.

- Impurity types and concentration as well as compound formation can significantly affect hydrogen isotope recycling and overall performance of plasma operation.

- Mixed materials effects in future large devices will impact hydrogen isotope recycling and affect plasma successful operations.

- Liquid metals as PFCs while offering great advantages in heat removal and plasma operation, care and detail surface and chemistry analysis are needed to assess the full behavior in real and extended reactor operation.