

Calculations of Helium Bubble Evolution in the PISCES Experiments with Cluster Dynamics

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APS-DPP meeting, October 26, 2017

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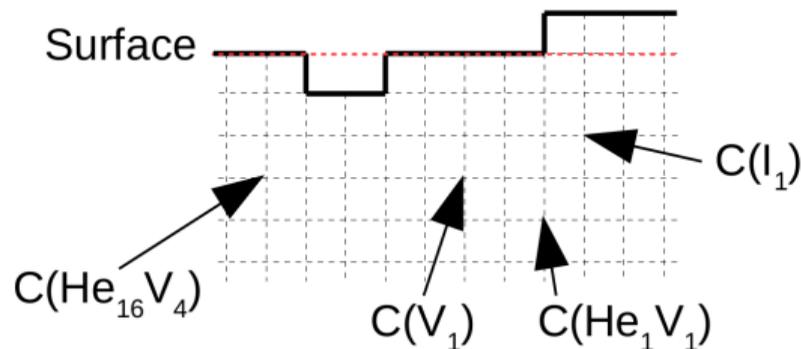
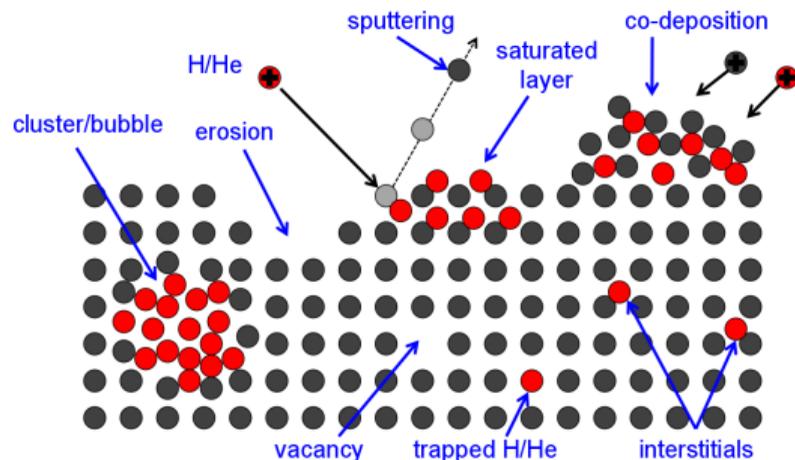
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The Material Model

The tungsten material is represented by the concentration of clusters at each spatial grid point:

- **Interstitials:** atoms of tungsten that are no longer on a lattice site
- **Vacancies:** missing atoms of tungsten on a lattice site
- **Helium:** helium atoms that are irradiated
- **Mixed:** combination of helium atoms trapped in tungsten vacancies



Reaction-Diffusion Equations

$$\delta_t \bar{C} = \phi \cdot \rho - \nabla \bar{J} - \bar{Q}(\bar{C})$$

- ▶ $\phi \cdot \rho$ is the incoming flux, the helium distribution profile is obtained from SRIM or MD simulations
- ▶ $\bar{J} = -D \nabla \bar{C}$ is the Fickian diffusive flux, with D_i following the Arrhenius equation

$$D_i = D_{0,i} e^{-E_m/k_B T}$$

with $D_{0,i}$ and E_m obtained from MD and DFT simulations

- ▶ $\bar{Q}(\bar{C})$ is the reaction term:

Production: $A + B \rightarrow E$

$$k_{A,B}^+ = 4\pi(r_A + r_B)(D_A + D_B)$$

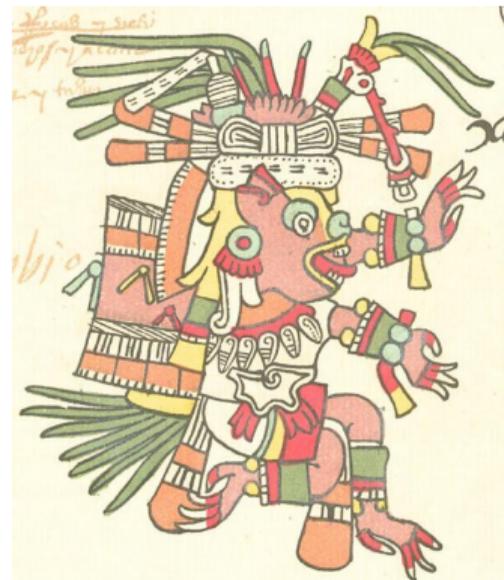
Dissociation: $F \rightarrow G + H$

$$k_{G,H}^- = \frac{1}{\Omega} k_{G,H}^+ e^{-\frac{E_b}{k_B T}}$$

- the capture radii r_i and the atomic volume Ω are calculated from geometric considerations and lattice parameter a_0
- the binding energy E_b associated to the dissociation is computed from the formation energies E_f given by MD and DFT simulations

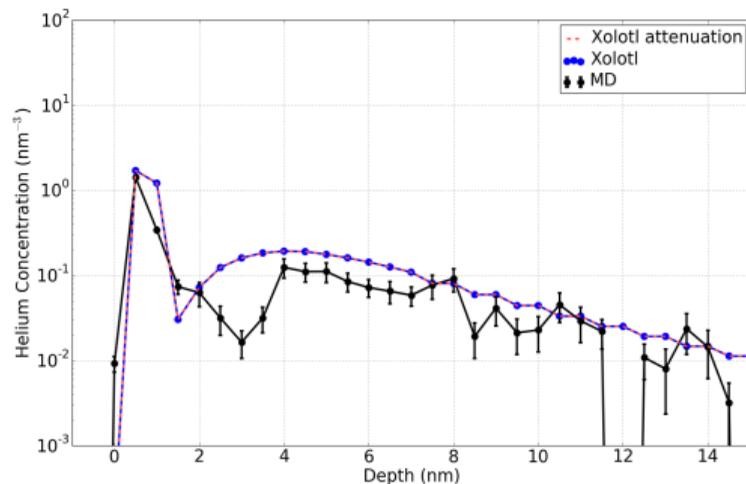
Xolotl

- ▶ Xolotl is the Aztec god of death and lightning
- ▶ Developed from scratch using C++ and MPI, designed by J. J. Billings (ORNL)
- ▶ The solver part (using PETSc developed at ANL) is independent of the physics part and it uses the finite difference approach
- ▶ A preprocessor creates the default options and kinetics needed to run Xolotl
- ▶ 2D/3D has been implemented
- ▶ Open source code available at <http://sourceforge.net/projects/xolotl-psi/>

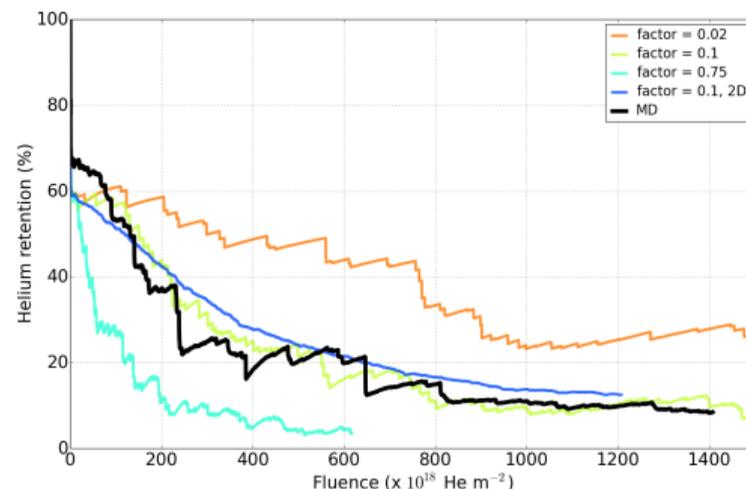


Benchmarking Xolotl with MD Simulations

Helium population as a function of depth for $4.0 \cdot 10^{25} \text{ He m}^{-2} \text{ s}^{-1}$ at 933 K at a fluence of $5.0 \cdot 10^{18} \text{ He m}^{-2} *$

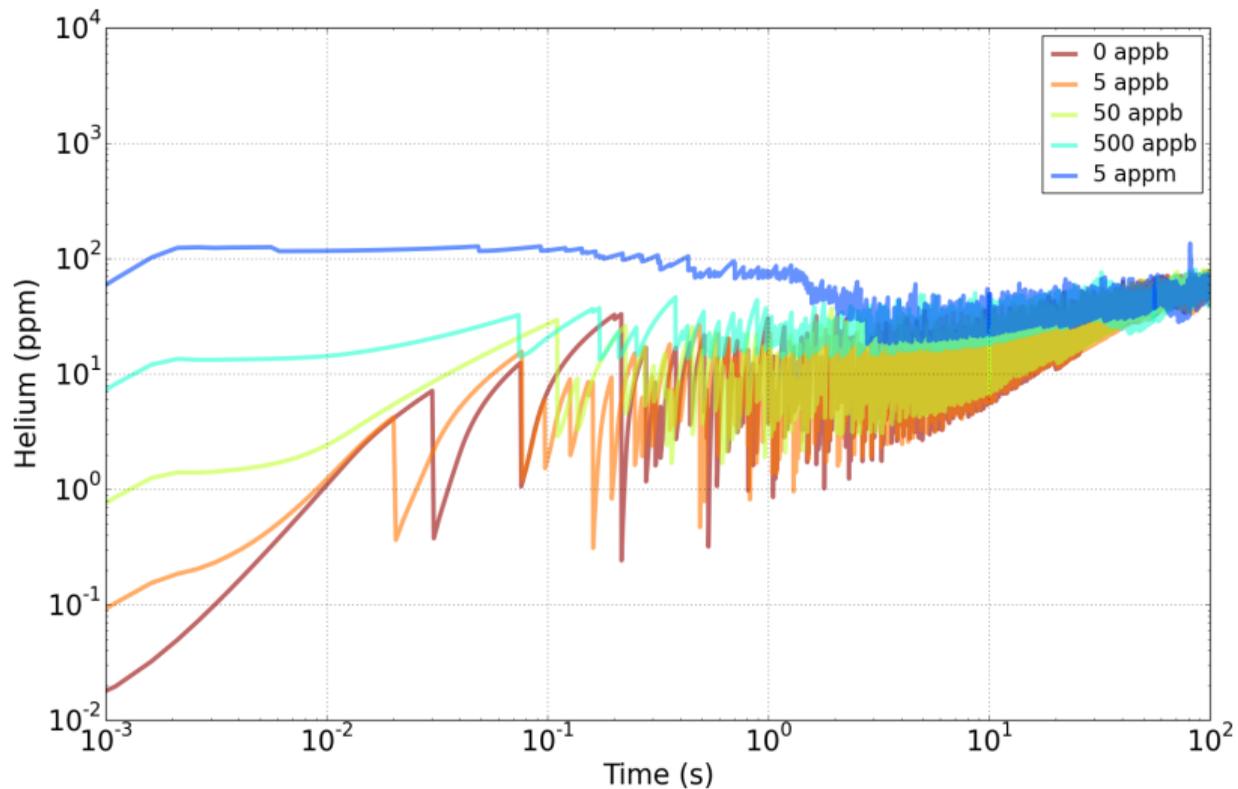


Helium retention evolution for $5.0 \cdot 10^{27} \text{ He m}^{-2} \text{ s}^{-1}$ at 933 K with bubble bursting



*Blondel *et al.*, Fusion Sci. Technol. 71, 22-35 (2017)

Bridging to Experiments (Preliminary)

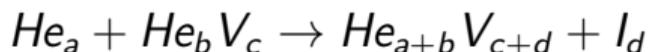


Flux: $4 \cdot 10^{22} \text{ He m}^{-2} \text{ s}^{-1}$ at 1170 K.

Surface Evolution

Different physical processes contribute to the surface evolution under irradiation.

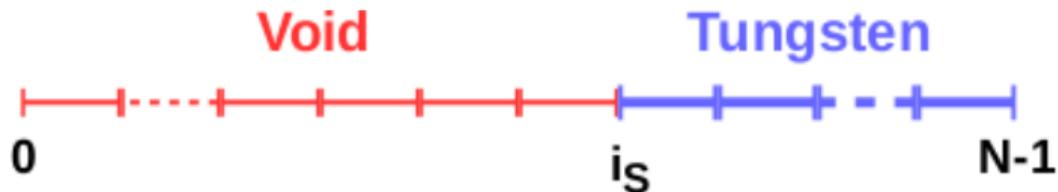
- ▶ **Trap mutation and loop punching:** When the bubble grows



These self-interstitials can then move to the surface and create adatoms (increase height).

- ▶ **Sputtering:** Tungsten atoms are ejected by incoming energetic particles (decrease height).
- ▶ **Re-deposition:** These tungsten atoms can then travel back to the material after ionization in the plasma sheath (increase height).

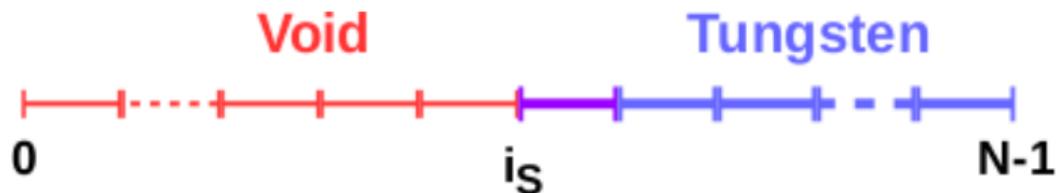
Surface Evolution in Xolotl



- ▶ No reaction, diffusion, or anything on the void grid points, concentrations are forced to 0.0
- ▶ On the tungsten side, classic ADR equations
- ▶ Count the number of interstitials diffusing from the $i_S + 1$ grid point to the i_S grid point to account for adatoms from trap mutation
- ▶ Remove the number of sputtered atoms given by the sputtering yield (given by FTriDyn)
- ▶ Profile of implanted interstitial for re-deposition is given by FTriDyn with energetics from GITR

Surface Evolution in Xolotl

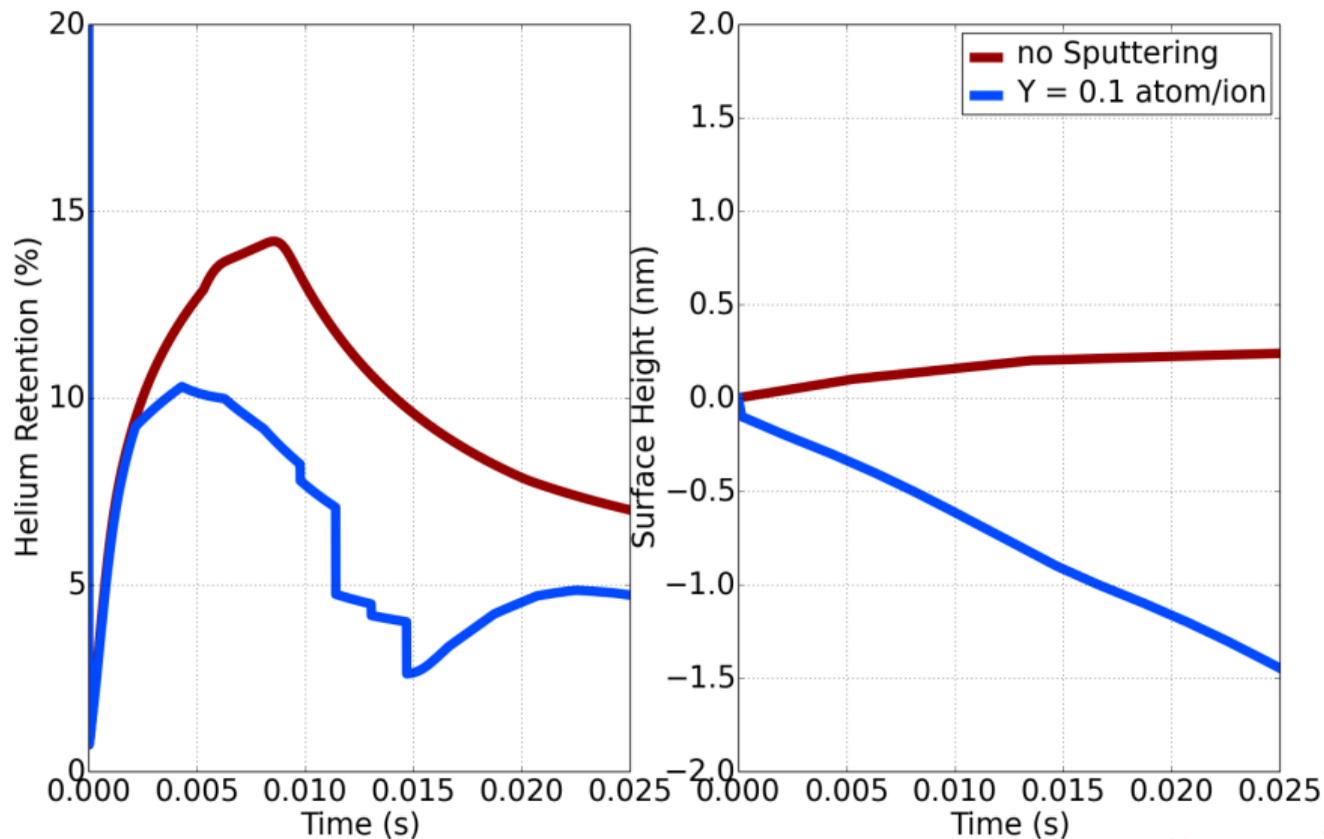
- ▶ When the interstitial flux at the surface reaches a given threshold (corresponding to the tungsten density), move the surface



- ▶ Re-initialize all the processes that are depth dependent (helium and re-deposition flux profiles, near-surface advection, near-surface trap mutation, ...)
- ▶ The surface can move up or down, by one or many grid points per time step

Results: Sputtering Effect

$4.0 \cdot 10^{22} \text{ He m}^{-2} \text{ s}^{-1}$ at 773 K.



Conclusion and Future Plans

- ▶ Tested effect of many parameters: flux, initial vacancy concentration, W re-deposition, sputtering yield, incoming helium energy, etc.

⇒ The coupling between Xolotl and FTriDyn (and GITR) behaves as expected.

- ▶ Short term plans:

- add the use of a bubble bursting model
- run 2D simulations with spatially dependent flux (see Ane Lasa presentation)

- ▶ Longer term plans:

- extend to helium-hydrogen irradiation

Thank You!