Effect of Helium Flux on Helium Accumulation in Near-Surface Tungsten

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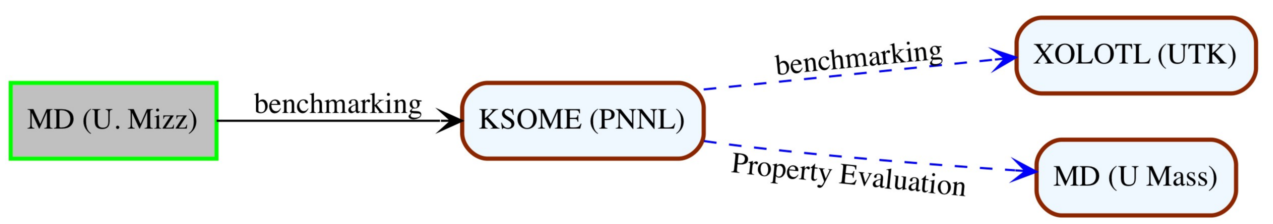
Motivation

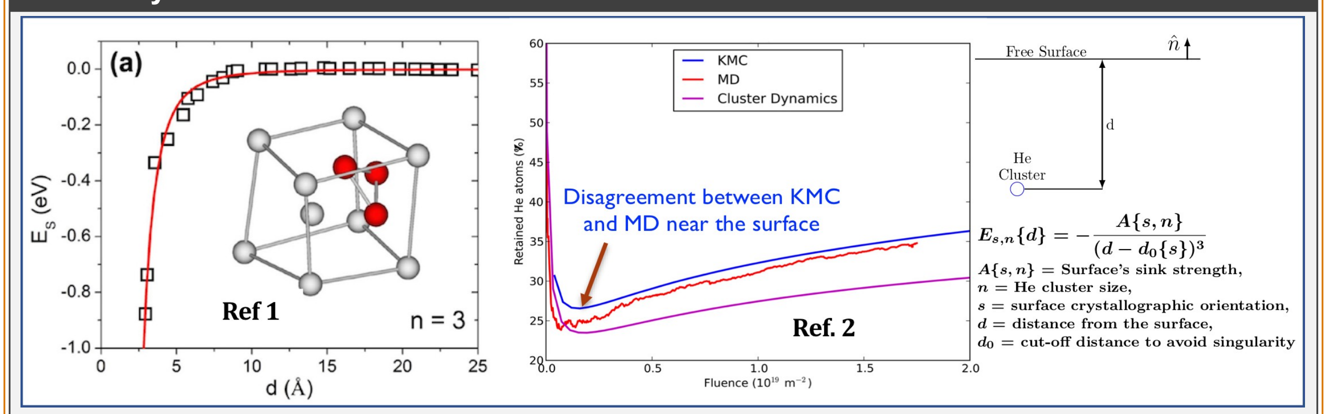
Provide experimentally relevant (~10^{21-24} He/m²/s) microstructure evolution due to He accumulation W subsurface for benchmarking the PFC simulator XOLOTL[a] and for MD evaluation of W thermomechanical properties for (100), (111) and (110) surfaces.

- Upgrade Object Kinetic Monte Carlo (OKMC) code KSOME[b]
- Perform longtime (>1 ms) under (a) isothermal conditions (Hmode) (b) and transient conditions corresponding to plasma ELMs
- Extending the time and length scales of KSOME (spatial decomposition and parallel processing)



KSOME Upgrade

Necessity



To incorporate:

- Biased He diffusion – subsurface region
- *Depth dependent* and *Depth specific* trapmutation rate

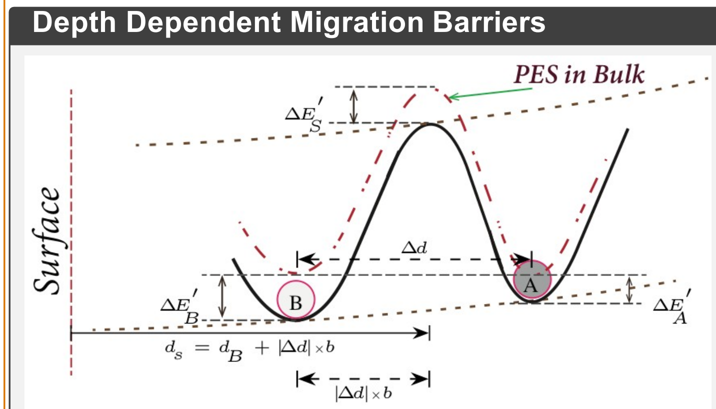
Note on KSOME Upgrades

To incorporate the effect of long range interaction of extended defects on point defect migration.

- Ability to parse mathematical expressions with basic math operations from a text file.
  Eg. To input functional forms for defect capture radii
- Calculate distance of point defects from geometrical objects.
  Eg. Surfaces, grain boundary, etc.

Simulation Details

Depth Dependent Migration Barriers



$$E^m_{A\to B}\{n,s,d\} = E^m_{bulk}\{n\} + \Delta E^m\{n,s,d\}$$

$$E^m_{A\to B}\{n,s,d\} = \Delta E'_S\{n\} + \Delta E'_A$$

$$\Delta E'_A = -A\{n,s\}\left[\frac{1}{(d_s-d_0)^3} - \frac{1}{(d_A-d_0)^3}\right]$$

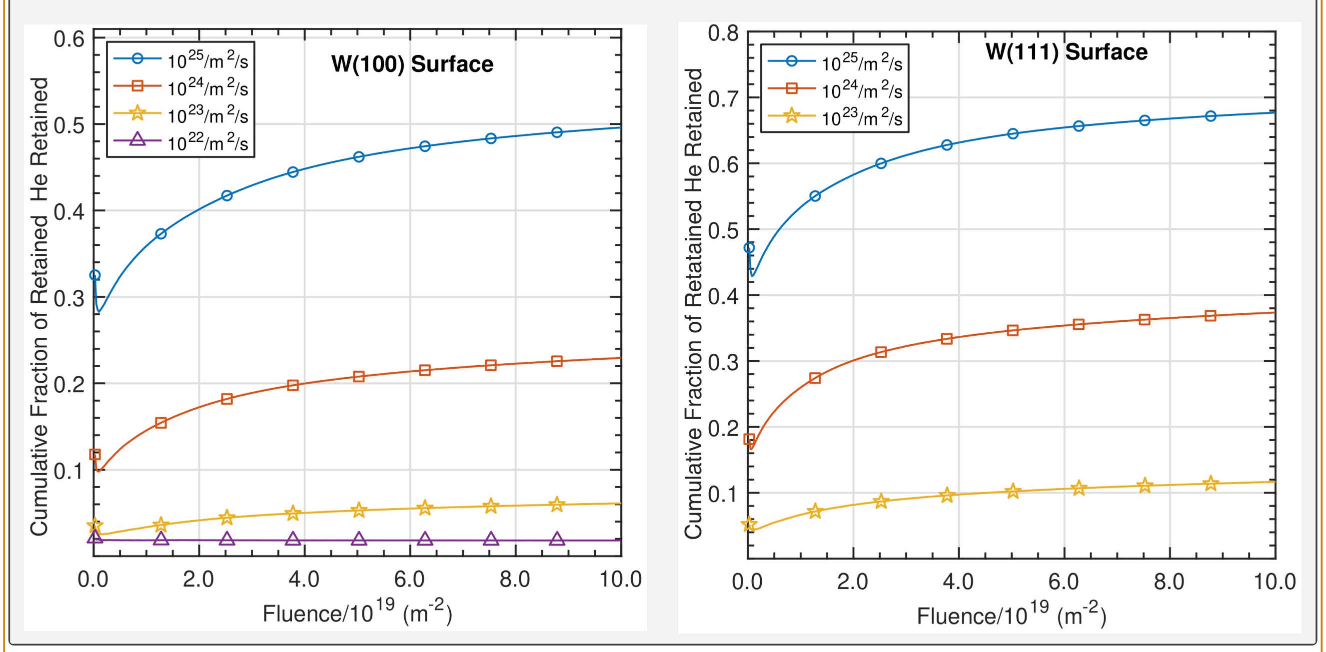
For the results presented here, $b = 0.5$, i.e the saddle point is midway between initial and final locations.

Simulation Parameters

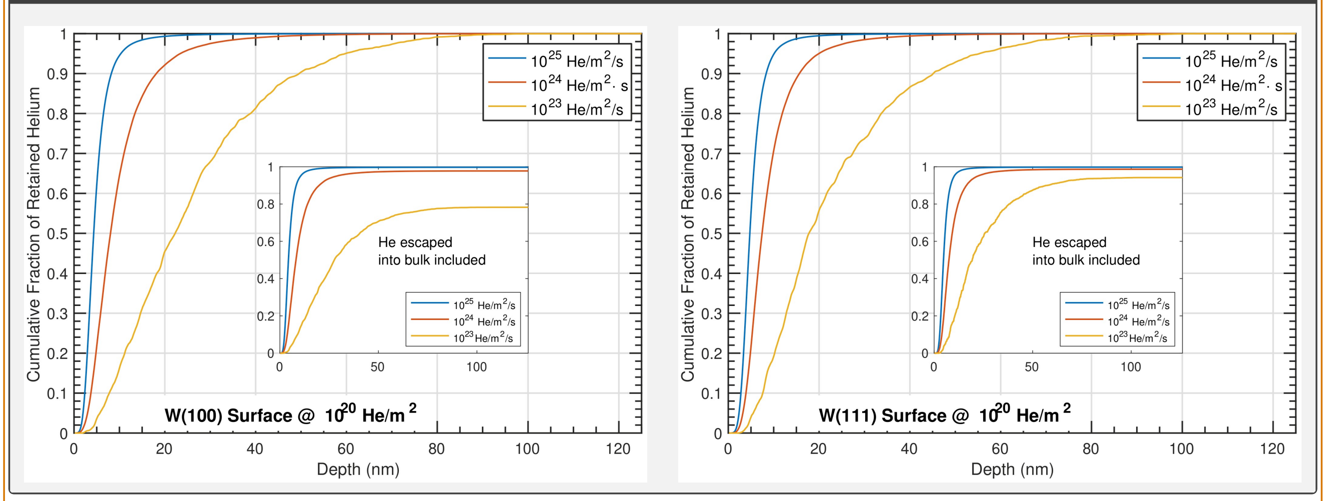
- Temperature = 933 K, He Energy = 100 eV
- Inbulk He Migration Parameter and capture radii were taken from Refs. 3 & 4, respectively
- Simulation Cell Dimensions: 254 × 254 × 127 nm³
- Surface dependent He implantation profiles obtained from MD simulations.
- Depth dependent trap mutation processes were NOT included.

Results

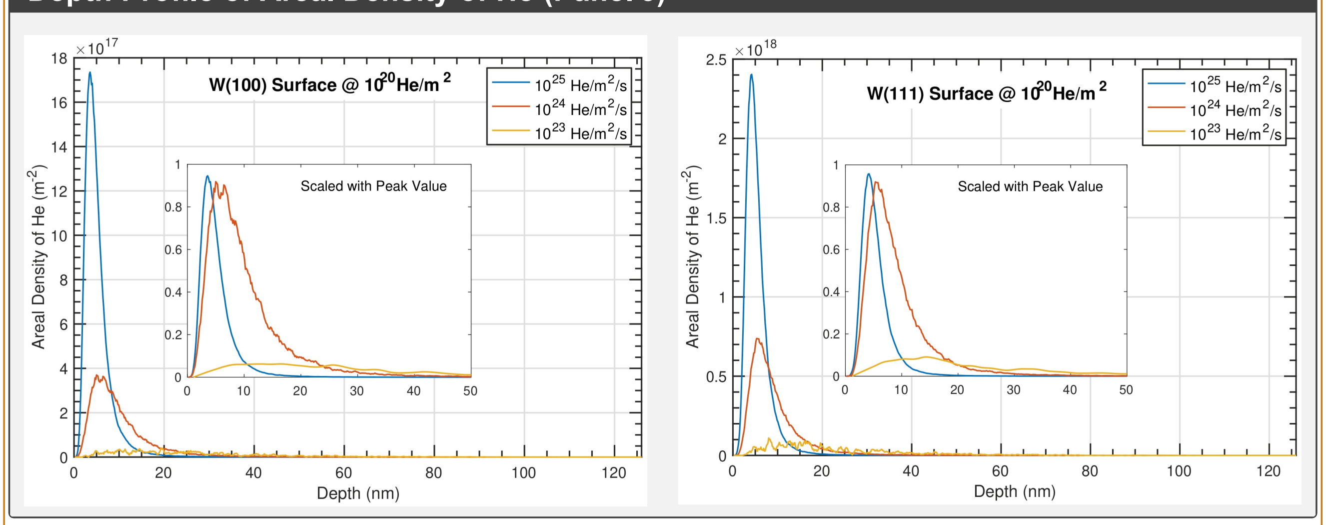
He Retention (Panel 1)



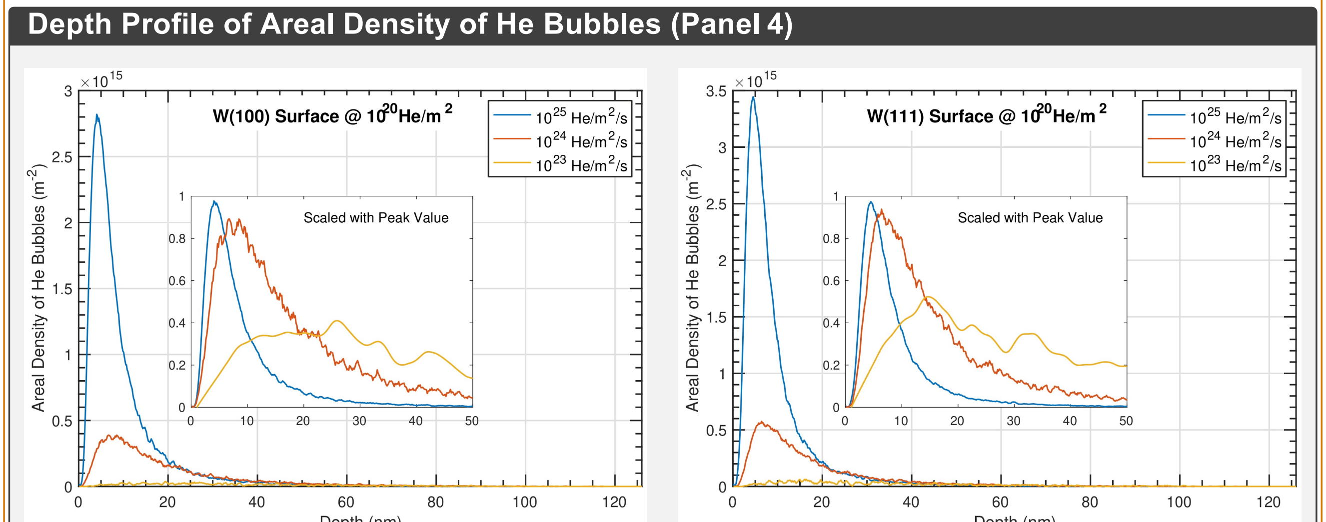
Cumulative Depth Distribution of He (Panel 2)



Depth Profile of Areal Density of He (Panel 3)



Depth Profile of Areal Density of He Bubbles (Panel 4)



Discussion

Qualitative behavior of He accumulation with *decreasing flux* for (100) & (111) surfaces is same

- Retention decreases and becomes constant with fluence at low flux. (Panel 1)
- The same behavior is expected when the depth dependent trap mutation events are included. However, lowest flux required for the same behavior also decreases.
- He accumulation shifts away from the surface and into the bulk (Panels 2-4).
- The depth distribution of areal densities become less peaked and more broader. This shift is drastic when the flux is lowered from 10^{24} to 10^{23} He/m²/s.

Differences

- Retention for (111) surface is higher (Panel 1).
- Cumulative depth distribution of retained He within the simulation cell appear to be close to each other. (Panel 2) However, the fraction of retained He escaping into the bulk with decreasing flux is higher for (100) surface.
- It is likely of the difference in the He accumulation between (111) and (100) surfaces is due to the differences in the He implantation profiles (not shown)

References

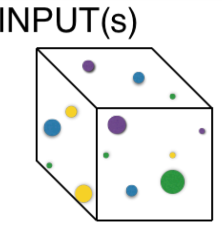
1. D. Maroudas et al, *J. Phys.: Condens. Mater.* 28 (2016) 064004
2. Z. Wang, et al, *Fusion. Sci. Tech* 71 (2016) 60
3. D. Perez, et al, *Phys. Rev B.* 90 (2014) 014102
4. C. Becquart et al, *J. Nucl. Mater.* 403, 75 (2010)

a. XOLOTL: Continuum reactiondiffusion cluster dynamics code
b. KSOME: Kinetic Simulations of Microstructural Evolution, an OKMC code

Acknowledgments This work is supported by the U.S. Department of Energy, Office of Fusion Energy Sciences and Advanced Scientific Computing Research (ASCR) through the SciDAC4 program.

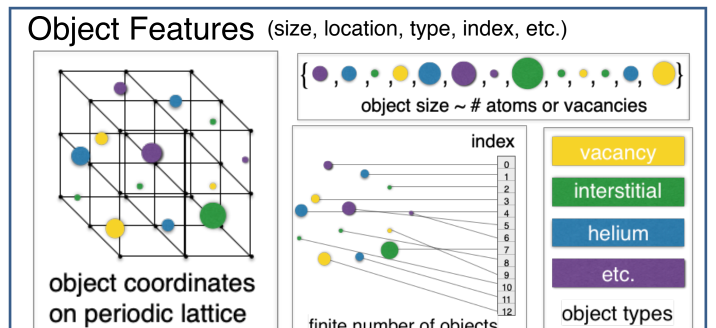
Computer Evaluation of OKMC

INPUT(s)



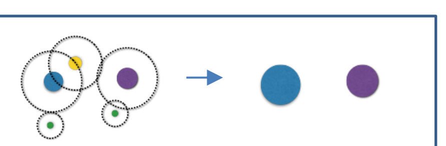
- file (production approach)
  - volume (nm^3), temperature (~1000 K), configuration of objects (molecular dynamics or DFT)
- quick start
  - <volume> <types> <time or max steps> <temperature>

Object Features (size, location, type, index, etc.)



Move Functions: Relations between objects are physical processes

- Reaction events (Capture, Annihilation, etc.)
- Diffusion



Algorithm (sequential by nature)

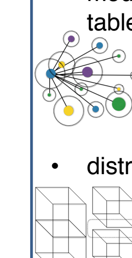
```
Input: object configuration, observables, rate functions
+0. process object reaction events to steady state
++ for each object: form reaction event list
++ decide reaction event based on minimum value search (distance between objects tie-breaker)
+++ if capture, update object size, diffusion prefactors, etc.; remove captured object from global state table
+++ if annihilate, remove both objects from global state table

+1. diffuse -sets time step size
++ for each object type: evaluate rate fractions and total rates; evaluate global system 'rate' (reduction to scalar value)
++ Monte Carlo step: randomly select object and orientation for diffusion; update global state table

+2. bump time and return to +0., or halt
```

Implementation Issues

- accessing and modifying global state 'table'
  - indices refer to the features for specific object in set of arrays - unordered lists of dynamic length
  - highly non-uniform memory access
- searches and 'table' updates dominate reaction events and are not FP dominated
- threaded programs in shared memory process models require atomic control of asynchronous global table updates and rate computations (reductions)
  - list formation, list orderings / searches, rate computations, etc. –threaded
  - Pthreads for symmetric multiprocessor CPUs; CUDA for streaming multiprocessor GPUs
- distributed memory required for larger volumes
  - resolve events at domain boundaries
  - resolve global time from local domain time (backtracking)



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