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

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Motivation

Provide experimentally relevant (~10²¹–²⁴ He/m²s) microstructure evolution due to He accumulation W subsurface for benchmarking the PFC simulator XOLOLT and for MD evaluation of W thermonic properties for (100), (111) and (110) surfaces.

Results

Necessity

Upgrade Object Kinetic Monte Carlo (OKMC) code KSOME²

- 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

To incorporate:
- Biased He diffusion - subsurface region
- Depth dependent and Depth specific trapping 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.
- E.g. Input functional forms for defect capture radii
- Calculate distance of point defects from geometrical objects.
- E.g. Surfaces, grain boundary, etc.

Simulation Details

Depth Dependent Migration Barriers

Depth dependent migration barriers will result in generalisability of our KSOME results. Here, we consider both surfaces and bulk.

Simulation Parameters

- Temperature = 333 K; He Energy = 100 eV
- Inbuilt 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 migration processes were NOT included.

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 10¹⁹ He/m²s.

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


XOLOLT: Continuum reactiondiffusion cluster dynamics code
KSOMMC: 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 SciDAC program.

Computer Evaluation of OKMC

Object Features

- object coordinates on periodic lattice
- quick start
- configuration <type> (volume or line): <temperature>

Move Functions: Relations between objects are physical processes
- Reaction events (Capture, Annihilation, etc.)
- Diffusion

Algorithm (sequential by nature)

Input object configuration, desired time frames
- Process object reaction events to steady state
- For each object: from reaction event list
- Decide reaction event based on minimum total energy between sources and sinks; perform reaction, remove captured objects from global state table
- If available, remove both objects from global state table
- Diffuse - next time step size
- For each object type, perform diffusion and total state evaluate global state table
- For each object type, perform diffusion and total state evaluate global state table
- Move object step: randomly select object and interaction for diffusion update global state table

Implementation issues

• Accessing and modifying global state: ‘table’
• Increase 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 approaches in shared memory process models require atomic control of asynchronous global table updates and race computations (reductions)
- List formation, list ordering / searches, rate computations, etc.- threaded

CPUs for symmetric multiprocessor (SPUs)
GPU for streaming multiprocessor (SPUs)
- Distributed memory required for larger volumes
- Display events at domain boundaries
- Resolve global time from local domain time (backtracking)

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