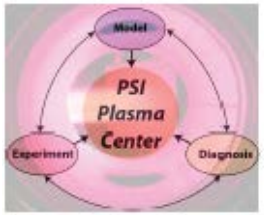
SciDAC-PSI: Plasma Surface Interactions Involving He

Brian D. Wirth*,#, on behalf of

Institution	Principal Investigator	Additional Personnel
ANL	Barry Smith (FASTMath)	Vijay Mahadevan (FASTMath)
GA/DIII-D	Vincent Chan	Rui Ding, Adam McLean (LLNL)
LANL	Xianzhu Tang	Jim Ahrens & Li-Ta "Ollie" Lo (SDAV), David Higdon (QUEST), Danny Perez, Luis Sandoval, Art Voter, Blas Uberuaga
ORNL*	**Brian Wirth***	Alexander Barashev, **David Bernholdt**,** Jay Jay Billings, Sophie Blondel, John Canik, Crystal Jernigan, Jeremy Meredith (SDAV), Phil Roth (SUPER), Roger Stoller
PNNL	Rick Kurtz	Giridhar Nandipati, Ken Roche, Wahyu Setyawan
UCSD	Serge Krasheninnikov	Jerome Guterl, Roman Smirnov
UIUC	David Ruzic	Davide Curreli, Kishor Kalathiparambil, Kyle Lindquist, Ivan Shchelkanov
UMass-Amherst	Dimitrios Maroudas	Lin Hu
UTK	Brian Wirth	Mary Alice Cusentino, Karl Hammond, Donghua Xu

In partnership with



UMASS AMHERST
ILLINOIS
UCSanDiego
* bdwirth@utk.edu
THE UNIVERSITY of TENNESSEE KNOXVILLE

Presented at SciDAC-3 PI Meeting
Washington, DC

1 August 2014

GENERAL ATOMICS
DIII-D NATIONAL FUSION FACILITY

Argonne NATIONAL LABORATORY

Pacific Northwest NATIONAL LABORATORY

Los Alamos NATIONAL LABORATORY EST. 1943

#
OAK RIDGE National Laboratory

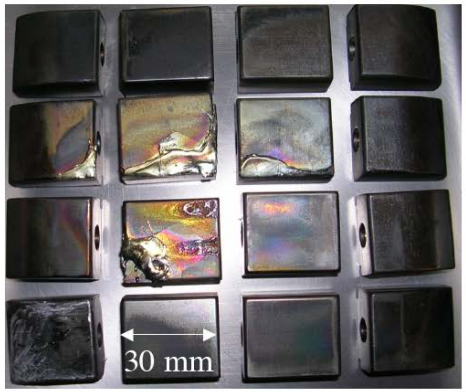
This work is supported by the U.S. Department of Energy, Office of Fusion Energy Sciences and Advanced Scientific Computing Research (ASCR) through the SciDAC-3 program.

The Challenge: No current materials are viable to bridge the significant gap between today's tokamaks & future fusion reactors

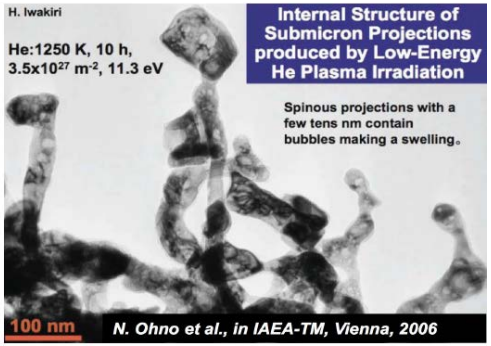
Issue / Parameter	Present Tokamaks	ITER	DEMO	Consequences
Quiescent energy exhaust *GJ / day*	~ 10	3,000	60,000	- active cooling - max. tile thickness ~ 10 mm
Transient energy exhaust from plasma instabilities $\Delta T \sim MJ / A_{wall}(m^2) / (1\ ms)^{1/2}$	~ 2	15	60	- require high $T_{melt/ablate}$ - limit? ~ 60 for C and W - surface distortion
Yearly neutron damage in plasma-facing materials *displacements per atom*	~ 0	~ 0.5	20	- evolving material properties: thermal conductivity & swelling
Max. gross material removal rate with 1% erosion yield *(mm / operational-year)*	< 1	300	3000	- must redeposit locally - limits lifetime - produces films
Tritium consumption *(g / day)*	< 0.02	20	1000	- Tritium retention in materials and recovery

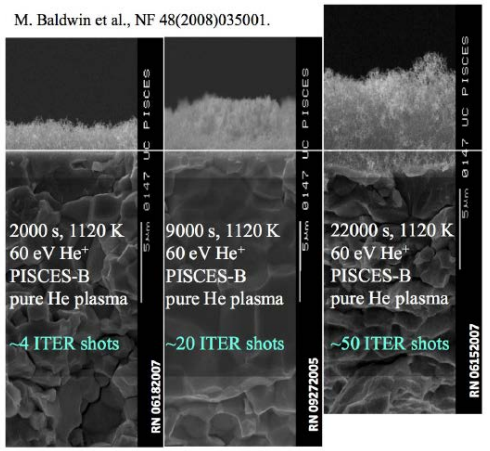
ITER's current operating plans involve (only) a tungsten divertor: significant current concern about sub-surface helium bubble formation & surface morphology changes that will influence core plasma performance & substantial tritium retention

C-Mod Molybdenum (T_{melt}=2900 K) limiter melted during disruptions



- Dilute MFE plasma (n~10^{20} m^{-3}) extinguished by small particulate
  - ➢ 2 mm "drop" of W == $N_{e,ITER}$





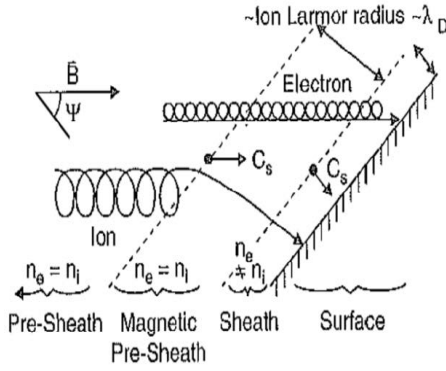
Plasma Surface Interactions (PSI) Objective

• Objective is to develop PSI simulation capability across three coupled spatial regions:

- **Edge/scrape-off-layer region of the plasma, with sheath effects**

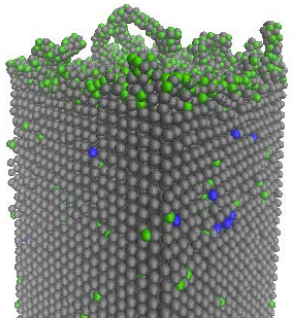
- **Near surface material response to plasma exhaust, with neutron damage and influenced/coupled to plasma sheath**

- **Structural materials response to intense, 14 MeV-peaked neutron spectrum**



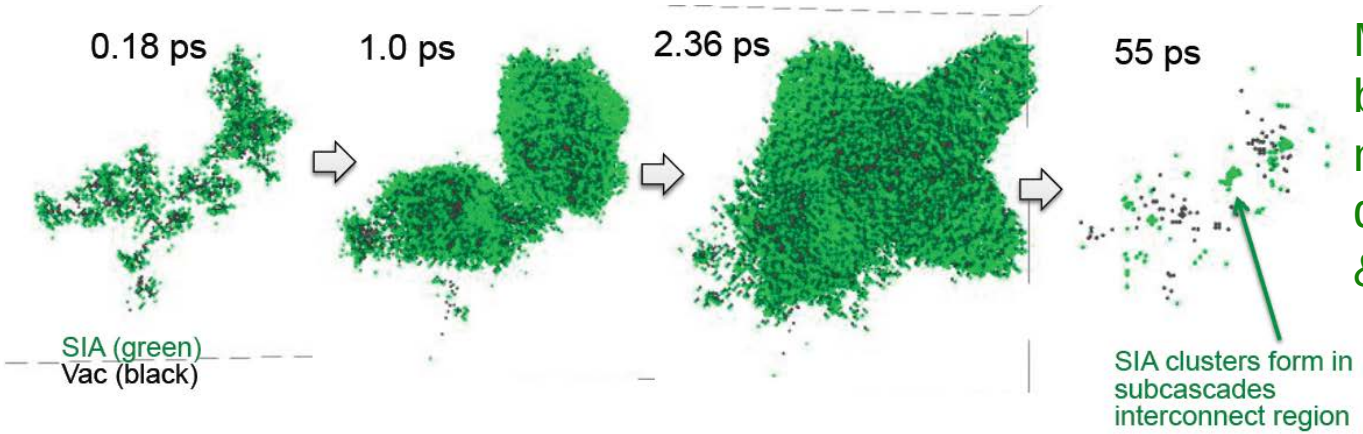
Plasma Edge SOL Sheath – heat & particle flux, recycling, etc.

mm



Material surface - erosion (impurity & dust), T retention, surface evolution

10^{2} – 10^{3} nm



Material bulk – neutron damage & transmutation

10^{-3} – 10^{2} mm

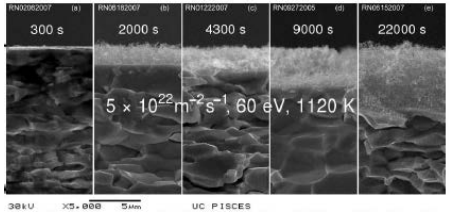
SciDAC – PSI Approach

• Developing simulation capability for plasma surface interaction across three coupled spatial regions:

- **Edge/scrape-off-layer region of the plasma (X. Tang, J. Canik)**
- **Near surface material response to plasma exhaust, with neutron damage and influenced/ coupled to plasma sheath (B.Wirth, B. Uberuaga, D. Maroudas)**
- **Structural materials response to intense, 14 MeV-peaked neutron spectrum (R. Kurtz)**
- **Experimental validation interface/database (V. Chan, D. Ruzic)**

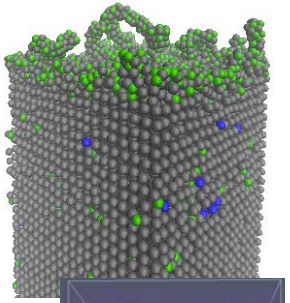
• Simultaneous ‘bottom-up’ and ‘top-down’ approach to multiscale modeling that integrates SciDAC institute capability into both particle and continuum based codes, and develops from scratch a new code, Xolotl for PSI

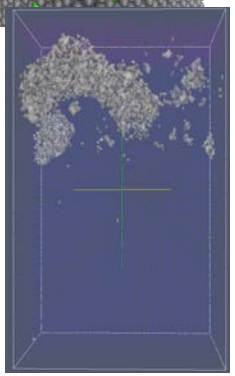
• Explore the ‘hand-shaking’ between plasma and materials models across these interfaces

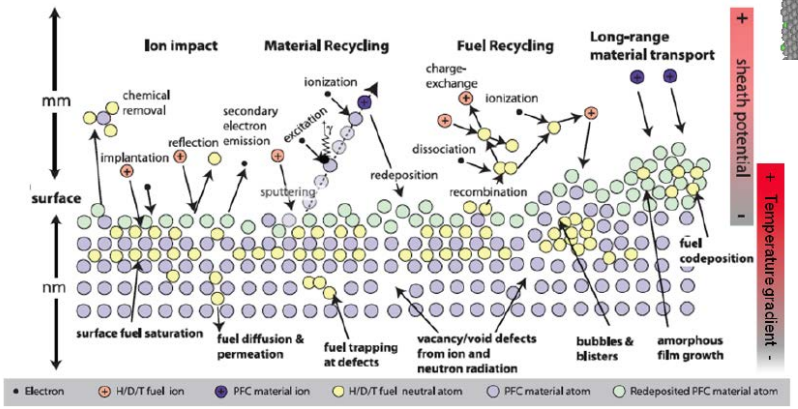


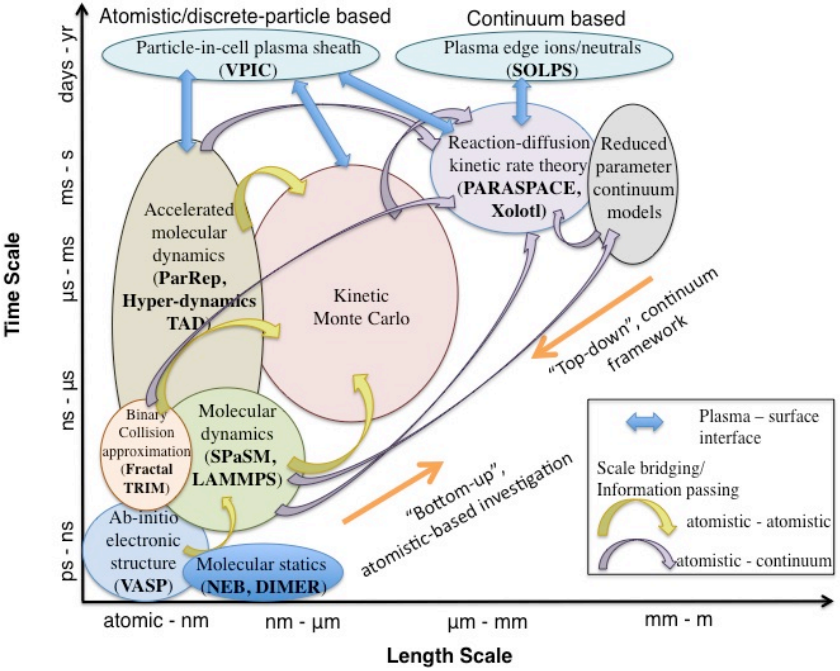
900 K < T < 1900 K

fuzz / coral

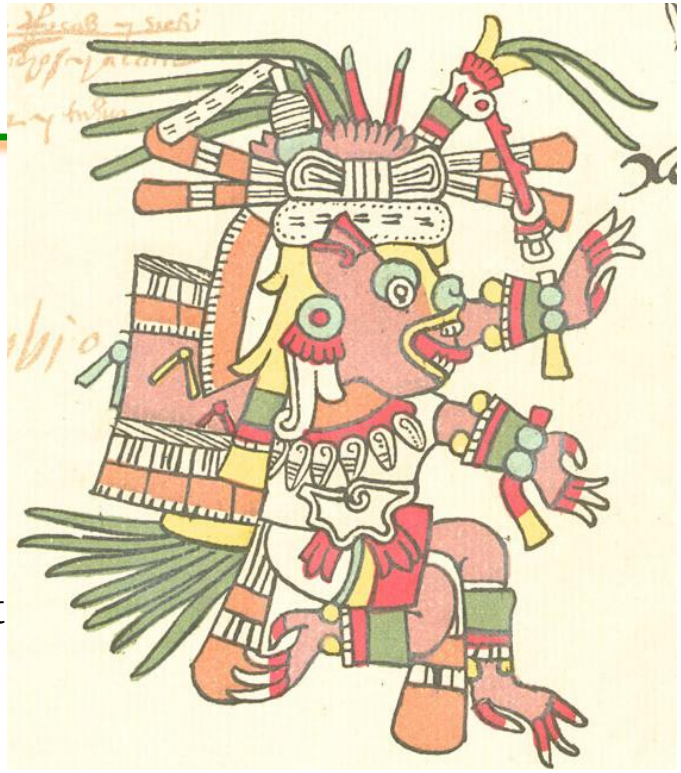








Xolotl:PSI*



- Xolotl (SHO-lottle) is the Aztec god of lightning and death
- Developed from 'scratch' for this project, designed for HPC current & emerging architectures (multicore, multicore + accelerator(s)) to solve advection – reaction – diffusion problems within a spatially resolved continuum domain:

$$\delta_t \bar{C} = \phi \cdot \rho + D\nabla^2 \bar{C} - \nabla \bar{\nu} C - \bar{Q}(\bar{C})$$

- Independent modules for physics, solvers, data management
- Developed in C++ with MPI for initial 1D finite difference
  - Approach to expanding dimensionality currently being reviewed
- Strong engagement with Institutes during code design and development
  - SDAV EVAL in situ analysis and visualization
  - SUPER GPTL built-in timing infrastructure
  - FASTMath PETSc-based solver, MOAB meshing
  - QUEST UQ Toolkit to model and propagate uncertainties in formation energies (inputs, obtained from MD simulations)
- Currently working on V&V and performance/scaling studies for He retention in W
  - Reviewing approaches to multi-threading and GPU utilization

* Available at http://sourceforge.net/projects/xolotl-psi/

SciDAC-PSI collaboration with FASTMath drives memory enhancements for reaction-diffusion modeling

Objectives

- Increase the number of clusters (degrees of freedom) modeled in reaction-diffusion-advection cluster dynamics to enable predictions of Tritium-He interactions with evolving defect microstructure in Fusion tokamaks, along with increasing spatial domain – critical for addressing ITER questions about tritium retention and permeation in divertor and plasma facing components

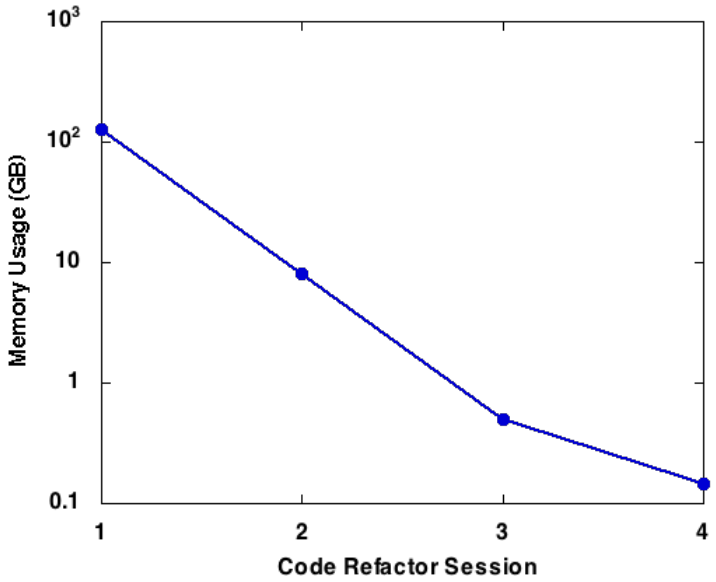
Impact

- Usable network size increased from $7x10^3$ to ~ $2x10^4$ clusters with sufficient memory for beyond 10^7
- Depth below the surface increased from 8 to 128 nm with sufficient memory for beyond 2500nm.
- Overall memory use decreased by 5000x from 128GB to 148MB

Approach

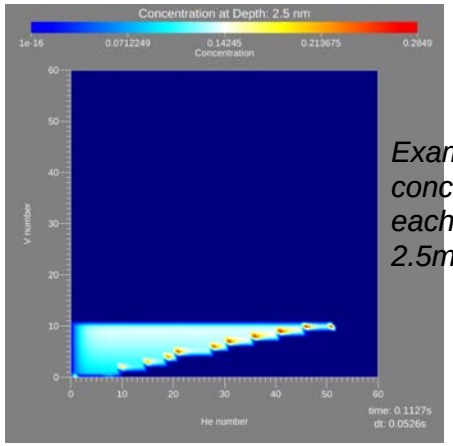
- Joint collaboration between FASTMath and SciDAC-PSI (Smith/PETSc team with Billings and Bernholdt/Xolotl-PSI team)
- Memory performance (Xolotl and PETSc) used to identify high memory use hotspots.
- Refactored the Jacobian matrices in PETSc to eliminate reliance on temporary matrices.
- Profiled Xolotl's heap to locate sparse arrays, extra data structures with Valgrind (--tool=massif option).
- Results committed into PETSc and Xolotl repositories

Memory usage decrease

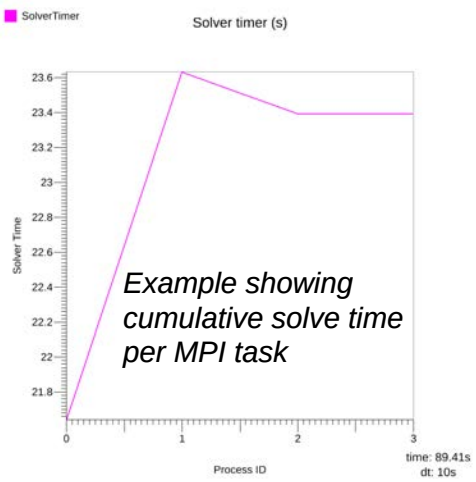


SciDAC-PSI collaboration with SUPER & SDAV incorporates performance timers & in-situ viz in Xolotl

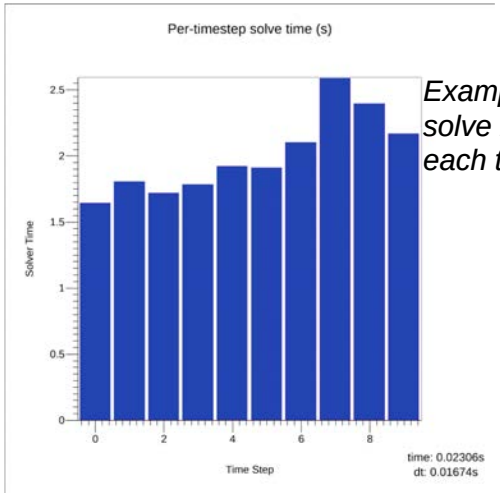
- Designed and implemented a lightweight, “always on” performance data collection infrastructure within XOLOTL
- Provides:
  - Timers: measure wall-clock time required to execute a specific part of the code
  - Event counters: count the number of times an event of interest occurs
  - Hardware counters: provide access to process hardware counters
- Uses General Purpose Timing Library (GPTL) and Performance Application Programming Interface (PAPI)
- Can be disabled with command line switch for lowest overhead
- XOLOTL has in situ scientific visualization and rendering capability using the Extreme-scale Analysis and Visualization Library (EAVL)
- Performance data, like science data, can be visualized using this capability



Example: concentration for each cluster type at 2.5mm depth



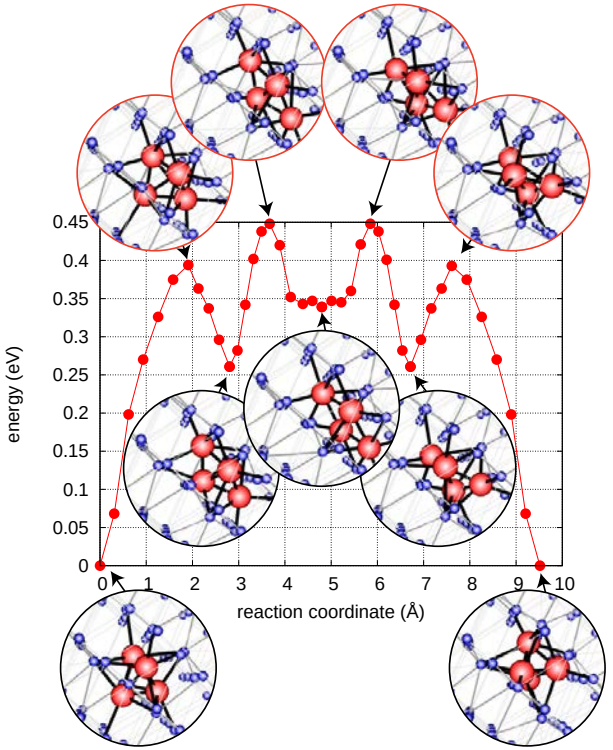
Example showing cumulative solve time per MPI task



Example showing solve run time for each timestep

*Thermodynamics & kinetics of small He clusters in W**

- Investigated the thermodynamics of small clusters containing between N=2 and 7 He
- Obtained kinetic parameters over a wide range of temperatures for:
  - Diffusivities, Breakup rates, Trap mutation rates, Capture radii
- Assessed different methods to obtain kinetic parameters



Main conclusions:

- Clusters become more stable with increasing size
- Diffusivities are strongly non-Arrhenius due to complex internal structure of clusters
- At operating temperatures, diffusivity does not significantly vary with size
- Breakup rate decreases with size; small clusters can dissociate rapidly
- Trap mutation rates strongly increase with size. For N=>5, mutation occurs faster than breakup.

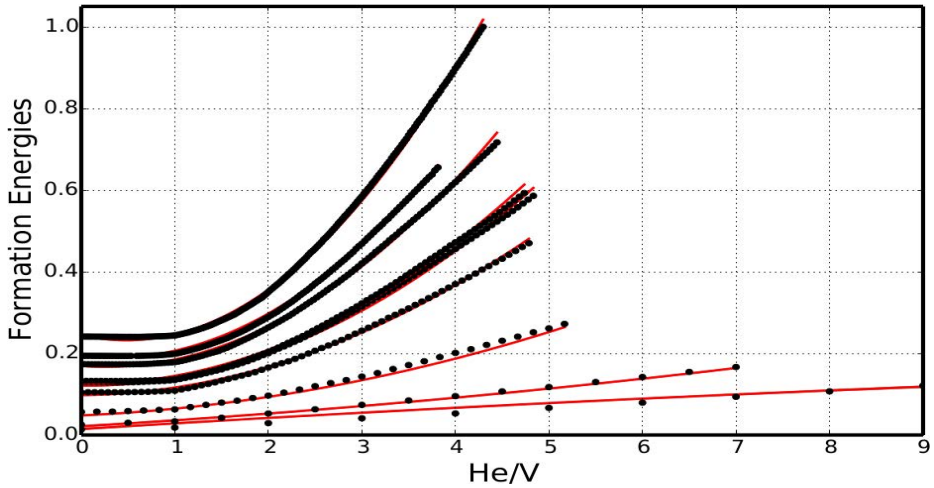
Main contribution: Provides thermodynamic-kinetic properties for continuum-cluster dynamics model (Xolotl)

* Perez, Vogel, and Uberuaga, *Diffusion and transformation kinetics of small helium clusters in bulk tungsten,* Phys. Rev. B (2014), in press

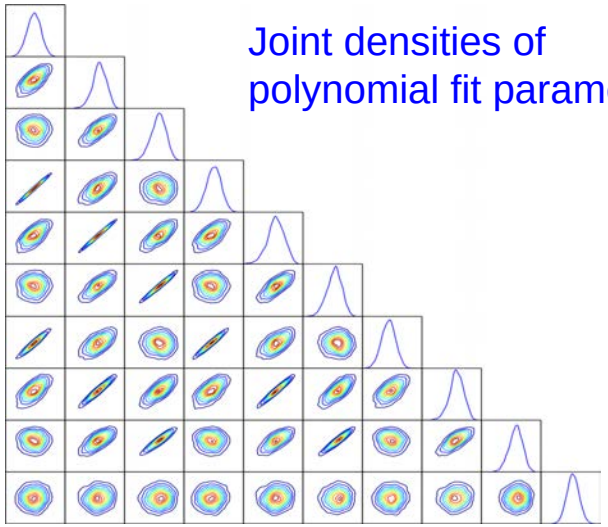
UQ activities in support of Xolotl-PSI

- Close collaboration with SciDAC QUEST, and using UQ toolkit (http://www.sandia.gov/UQToolkit/)
- Performed Bayesian inference, and polynomial chaos expansion to determine the sensitivities of Helium – vacancy cluster formation and binding energies using polynomial expansions to interpolate atomistic database

Atomistic database of cluster formation energy: f(V, He/V ratio)

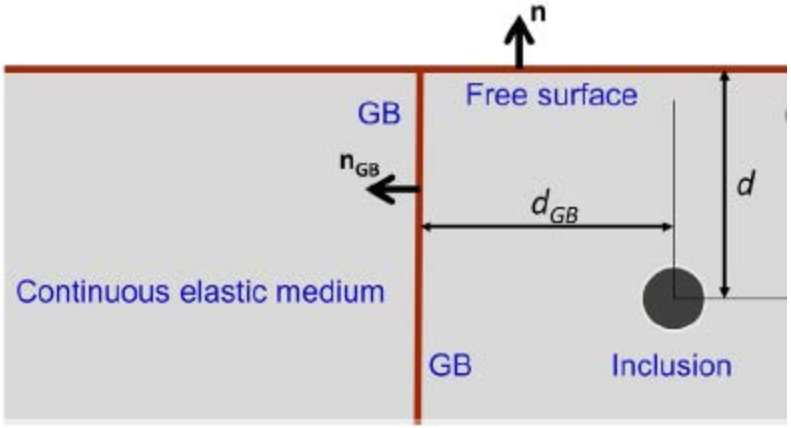


Joint densities of polynomial fit parameters



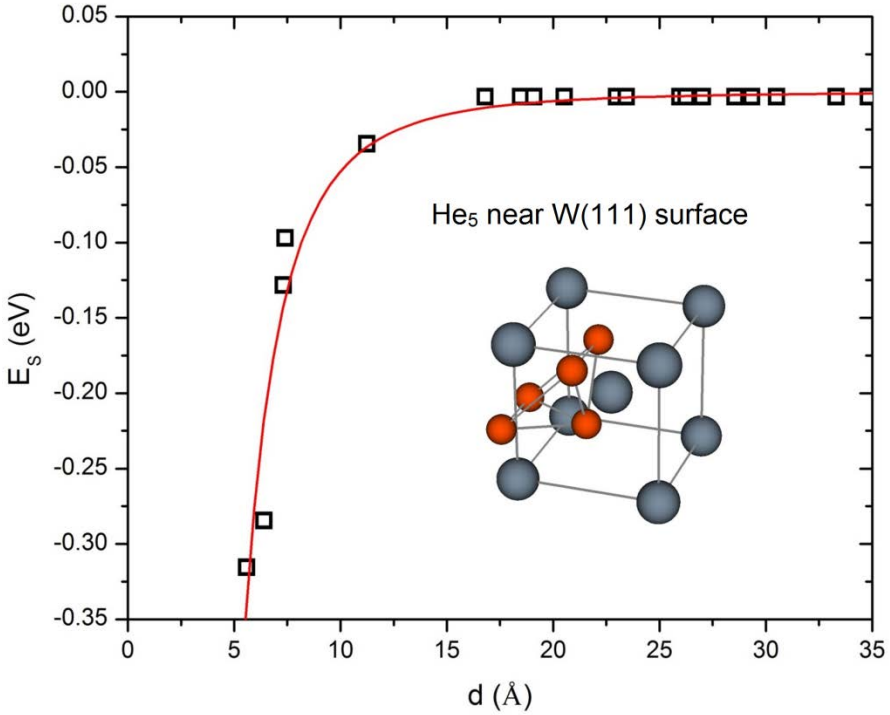
- Initial forward propagation of cluster formation energy variance through Xolotl has been performed
- Framework in place for Global Sensitivity Analysis
- Ongoing effort to provide detailed UQ analysis of influence of thermodynamic-kinetic cluster energetics impact on Helium retention and bubble distributions

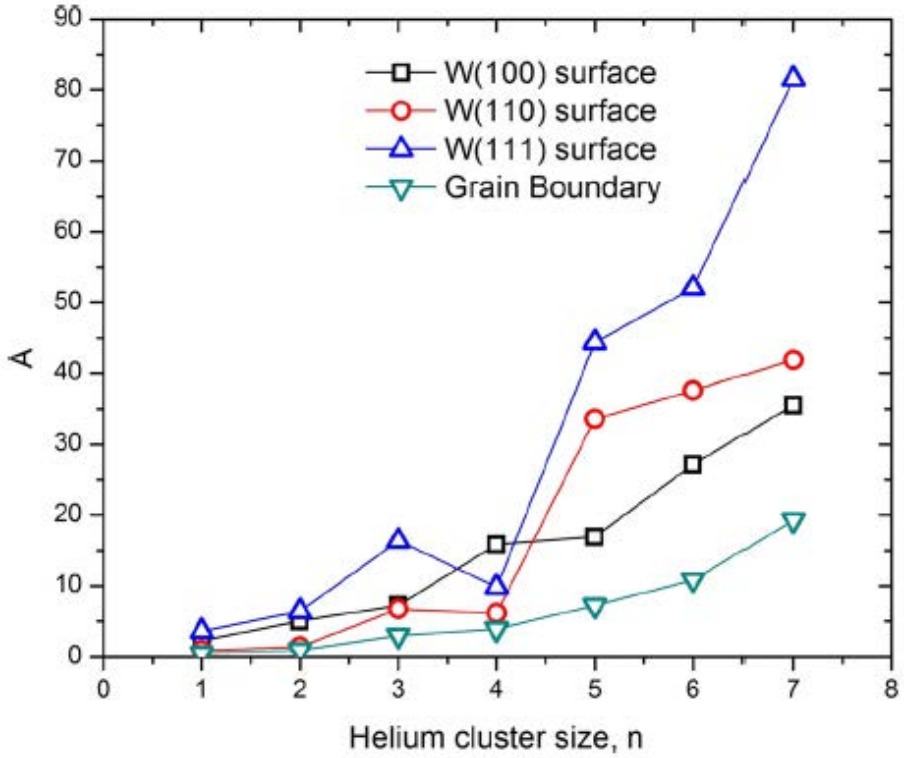
Atomistic study of He interactions with extended defects in W



$$U_i = E_{s,i}(d) = -\frac{A_{s,i}}{d^3}$$

$$U_i = E_{GB,i}(d_{GB}) = -\frac{A_{GB,i}}{d_{GB}^3}$$





- Elastic potentials (from elastic inclusion theory) parameterized according to molecular-statics (MS) simulations describe successfully He_n cluster-sink interactions in W
- He_n clusters ($1 \leq n \leq 7$) interacting with W(100), W(110), and W(111) surfaces and Σ3<111>{121} symmetric tilt GB examined
- Sink strength increases with cluster size

Hu, Hammond, Wirth, and Maroudas, *J. Appl. Phys.* **115**, 173512 (2014).

Summary of He interactions near surfaces

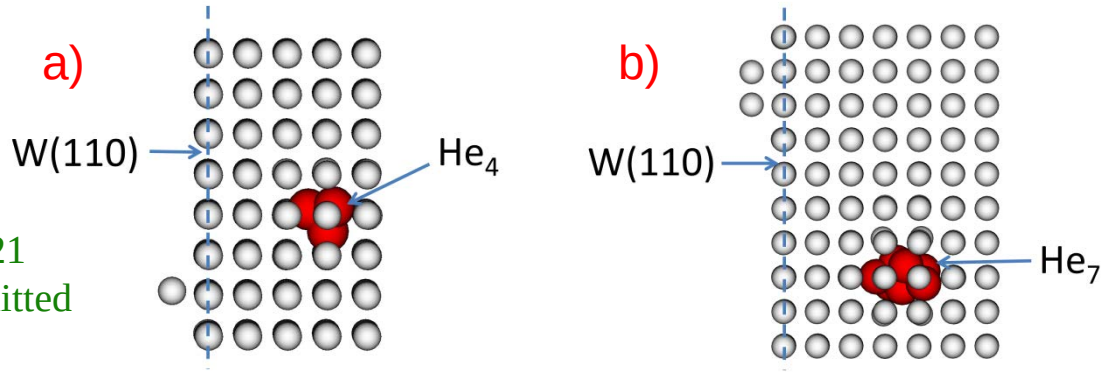
- Detailed analysis of several hundred MD simulations of each He_n cluster ($1 \leq n \leq 7$) dynamics near certain W(*hkl*) surfaces shows that cluster reactions dominated by trap mutation are activated as the clusters approach the surface at rates higher than in the bulk. A critical cluster size exists (n = 4-5) beyond which multiple W adatoms and vacancies form in trap mutation reactions.

Sink	He	He_2	He_3	He_4	He_5	He_6	He_7
W(100)	D (100%)	D (19.1%) PD (5.9%) TM (75.0%) 1 W_V	D (1.1%) PD (11.6%) TM (87.3%) 1 W_V	D (2.1%) PD (74.6%) TM (23.3%) 2 W_V	D (4.1%) PD (85.3%) TM (10.6%) 2 W_V	D (2.3%) PD (36.9%) TM (60.8%) 3 W_V	D (3.1%) PD (27.4%) TM (69.5%) 4 W_V
W(110)	D (100%)	D (31.6%) PD (1.3%) TM (67.1%) 1 W_V	D (0.0%) PD (2.0%) TM (98.0%) 1 W_V	D (0.0%) PD (0.0%) TM (100%) [a)] 1 W_V	D (0.0%) PD (0.0%) TM (100%) 2 W_V	D (0.0%) PD (0.0%) TM (100%) 2 W_V	D (0.0%) PD (0.0%) TM (100%) [b)] 2 W_V
W(111)	D (35.4%) TM (64.6%) 1 W_V	D (1.2%) PD (0.0%) TM (98.8%) 1 W_V	D (1.6%) PD (0.0%) TM (98.4%) 1 W_V	D (0.0%) PD (0.0%) TM (100%) 2 W_V	D (0.0%) PD (0.0%) TM (100%) 2 W_V	D (0.0%) PD (0.0%) TM (100%) 3 W_V	D (0.0%) PD (0.0%) TM (100%) 3 W_V

D: He Desorption
TM: Trap Mutation

PD: Partial Dissociation
W_V: Tungsten Vacancy

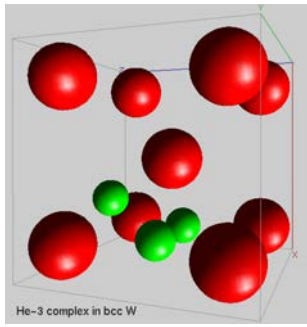
Hu, Hammond, Wirth, and Maroudas, *Surf. Sci.* **626**, L21 (2014); *J. Appl. Phys.*, submitted (2014).



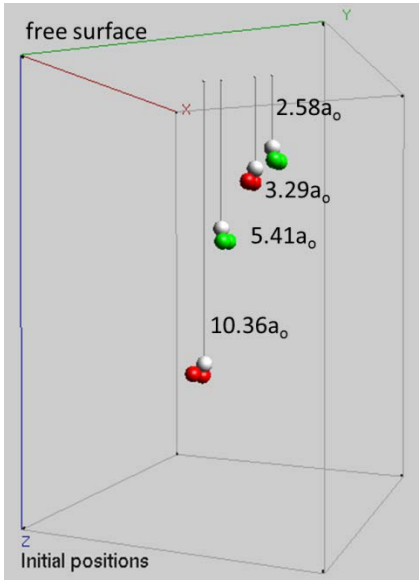
Behavior of small He clusters in W

Self-evolving atomistic kinetic Monte Carlo (SEAKMC) method employed to characterize behavior of small interstitial He and He-vacancy clusters in W.

- **The configuration of 3-He cluster geometry relative to free surfaces were investigated.**
- **Range of elastic interaction between surface and 3-He cluster is short-ranged (only a few lattice parameters) and weak, maximum binding energy of 0.3 eV at ~1 a_o from (110) surface.**
- **He interstitial clusters are highly mobile in the bulk, but immobilized by Frenkel pair formation when approaching free surface, creating immobile He-vacancy complex thru trap mutation that produces W interstitial that annihilates on surface, creating an adatom.**
- **Similar trap mutation (Frenkel pair) mechanism observed for He clusters far from surface but a larger number of He atoms required.**
- **Observed mechanisms can contribute to He retention in W components and tritium retention, if tritium is trapped in He-vacancy clusters. Adatom formation will produce changes in surface texture and may contribute to W 'fuzz' formation.**
- **SEAKMC results are similar to MD simulations performed within this SciDAC, although the impact of atomic vibrations near free surfaces may result in incorrect rates within the MC/SEAKMC simulations.**



Relaxed three-interstitial He cluster (green spheres) in a bcc W unit cell (red spheres)

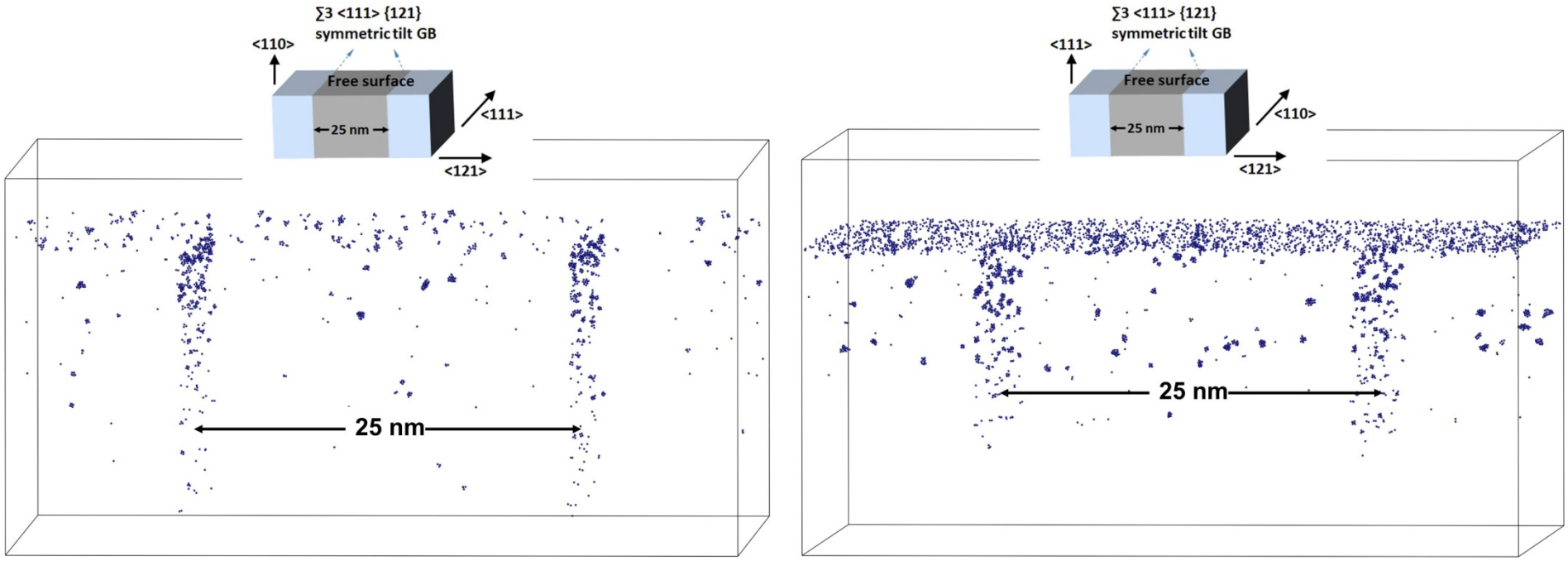


Initial cluster locations in SEAKMC simulations (a_o is W lattice parameter)

Barashev, Xu, and Stoller, J. *Nucl. Mater. submitted*

MD database demonstrates drift and segregation of He

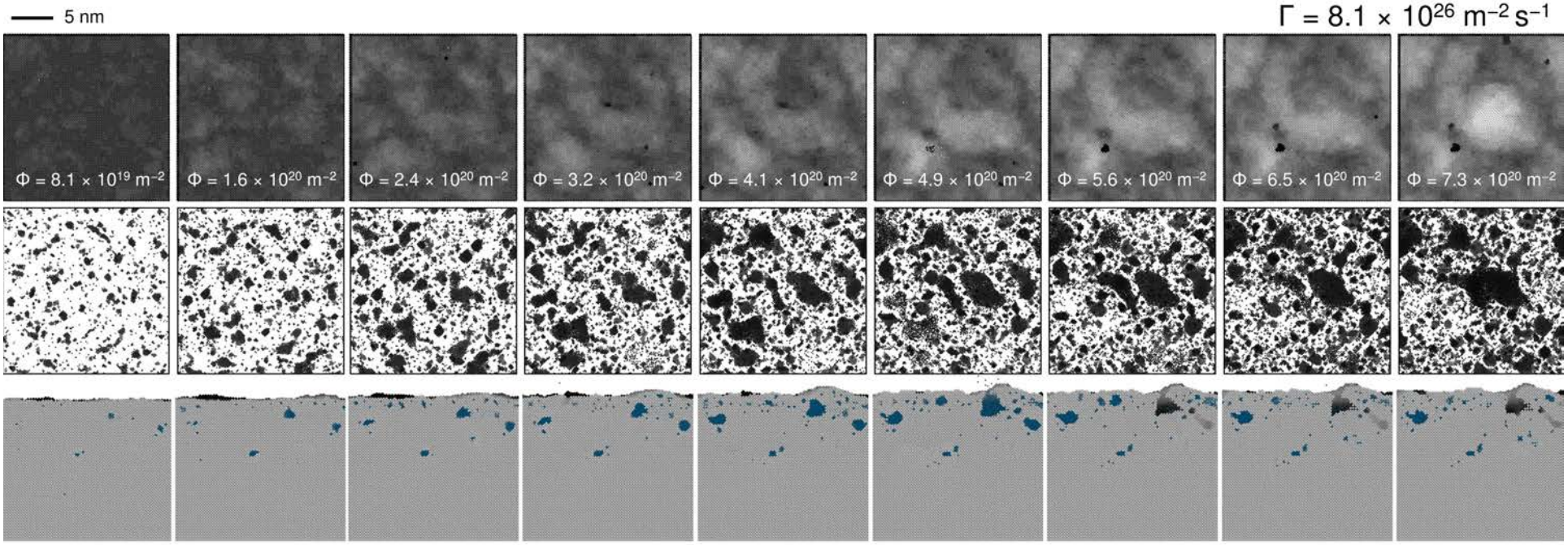
- Large-space-scale molecular-dynamics (MD) simulations (T = 933 K) of evolution of implanted He in model polycrystalline tungsten
- Simulations reveal helium aggregate formation and growth, as well as mobile He_n cluster diffusion, drift, and segregation on W surfaces and GBs
- Example: He distribution near GB intersections with W{110} and W{111} surfaces. Helium distribution determined by sink segregation strength, as well as trap mutation reactions that are activated as the clusters approach the sinks



Hu, Hammond, Wirth, and Maroudas, *J. Appl. Phys.* **115**, 173512 (2014).

MD database demonstrates bubble formation & surface evolution

- Large-space-scale molecular-dynamics (MD) simulations (T = 933 K) of evolution of implanted He in single crystalline tungsten
- Simulations reveal helium aggregate formation, growth, over-pressurization, trap mutation, and surface morphology evolution

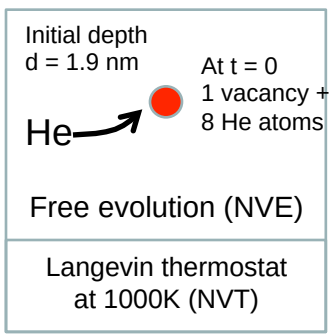


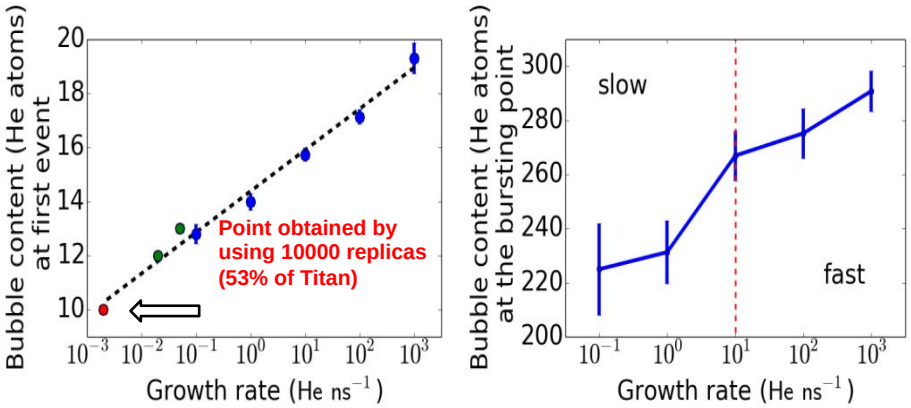
High-flux simulations showing surface growth and helium accumulation below a W(100) surface. Top: View of surface (white = +1.5 nm, black = –2 nm); Middle: helium atoms, top view (black = at surface, white = –15 nm); Bottom: cross-section.

Hammond and Wirth, manuscript in preparation.

He retention & He bubble growth in W: rate effects studied through MD & accelerated MD approaches

- He bubble growth* modeled by inserting He atoms within a pre-existing bubble at a given rate.
- Evolved using Parallel Replica Dynamics (ParRep) to reach growth rates that are orders of magnitude slower than MD.

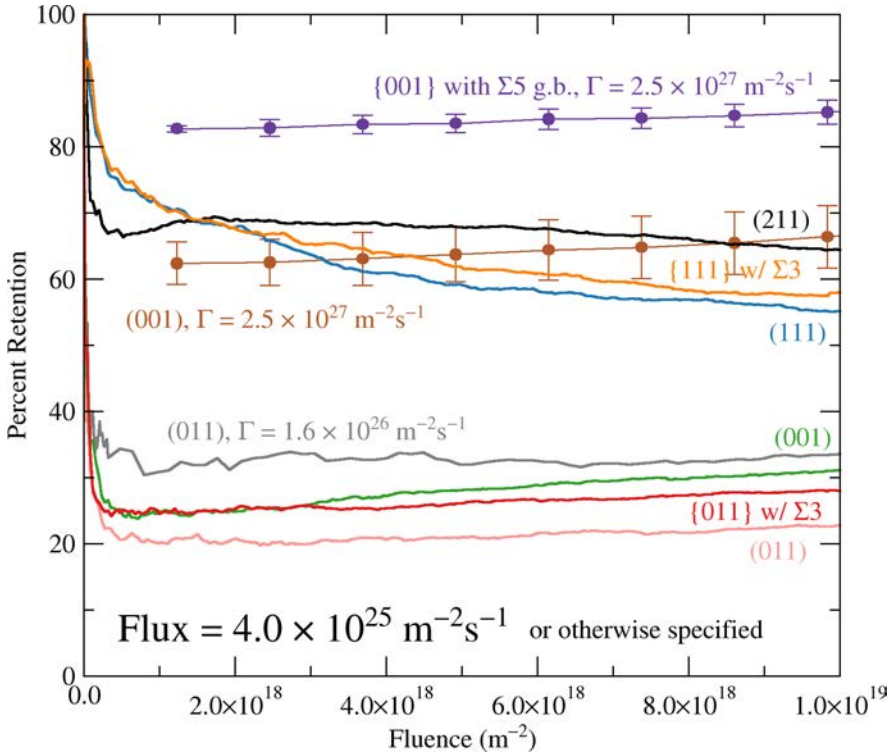




- At slow growth rates:
  - →The size/pressure at which W moves is much smaller.
  - →The size at which the bubble ultimately bursts is much smaller.

* Sandoval, Uberuaga, Perez, et al.

He retention in MD at 930-1200K**



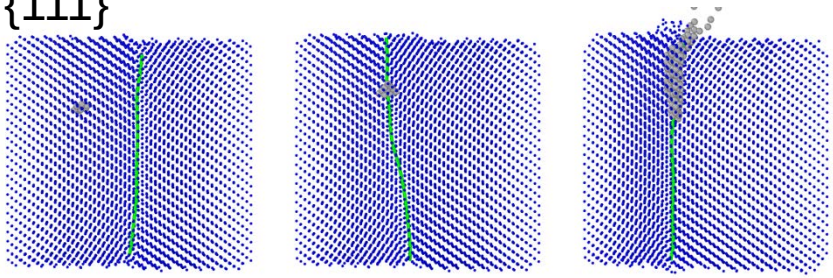
- Higher flux produces higher retention through He cluster 'self-trapping'
- {100}, {110} surfaces retain much less than {111}, {211} surfaces

** Hammond and Wirth *J. Appl. Phys.* **submitted**

Growth of He bubbles in W: extended defect influence

Screw dislocations

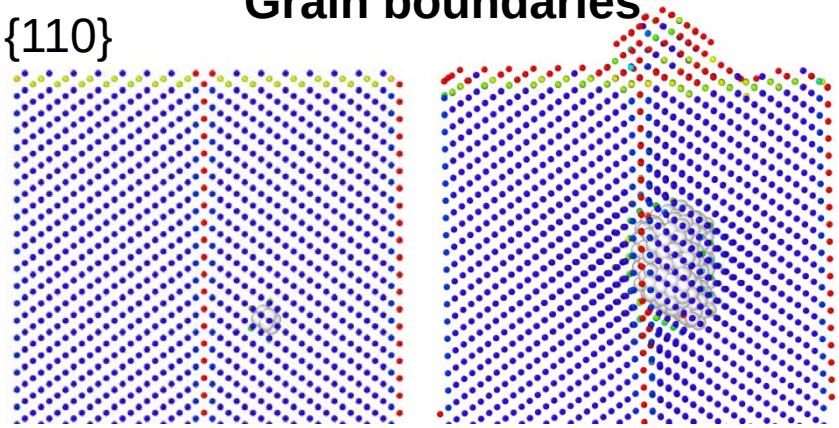
{111}



- Goal: Understand role of dislocations on He bubble evolution.
- The screw dislocation is attracted to the He bubble.
- Once the bubble touches the dislocation, it grows along it with an elongated shape.
- The screw dislocation becomes a path for the release of helium atoms.
- The process results in less damage as compared with the single crystal case.

Grain boundaries

{110}



- Goal: Understand role of grain boundaries on He bubble evolution.
- The grain boundary traps He clusters and acts as a nucleation center for He bubbles.
- Interaction between tungsten interstitials from Frenkel pairs and grain boundary.
- Grain boundaries considered:

  $\Sigma 3\langle 111\rangle\{121\}$, $\Sigma 3\langle 121\rangle\{111\}$

  $\Sigma 5\langle 021\rangle\{012\}$, $\Sigma 5\langle 031\rangle\{013\}$

Sandoval, Uberuaga, Perez, et al.

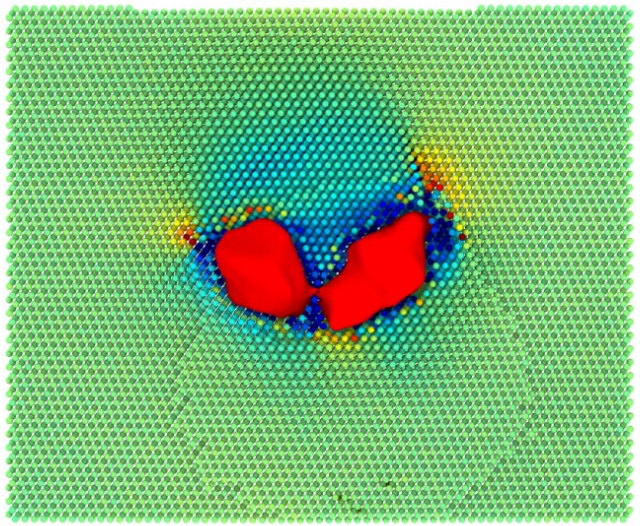
*Modeling He bubble coalescence**

- **Coalescence of He nano-bubbles proceeds by lateral growth of the bubbles due to formation of compression region between the bubbles and repulsive interaction of dislocation loops emitted towards each other**
- **The bubbles form common stress field and spanning dislocations, which are qualitatively similar to ones around a single bubble**
- **When resolved shear stress is not strong enough to punch dislocation loops, incomplete release of the loops can create dislocation dipoles and jogs leading to formation of long vacancy chains in slip directions as the loops are eventually released**
- **Precipitation of He on the vacancies can form chains of helium bubbles along 〈111〉 directions, which were observed experimentally in fuzz growth experiments [Miyamoto et al, *JNM 415 (2011) S657*]**

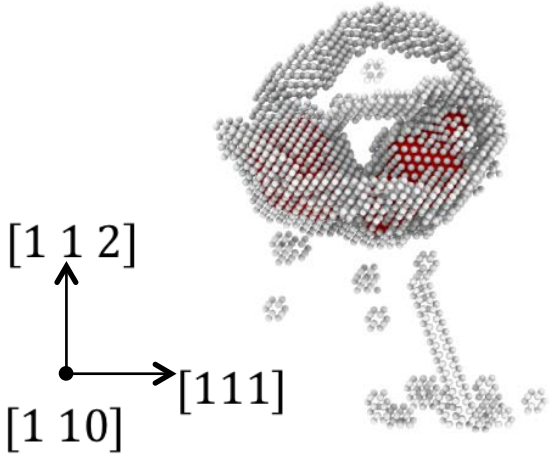
Simulated dynamics of He atoms and dislocations, generated by the growing bubbles, can play essential role in the fuzz formation

Smirnov, Krasheninnikov, and Guterl, *J. Nucl. Mater.,* submitted (2014).

Stress field around coalescing bubbles

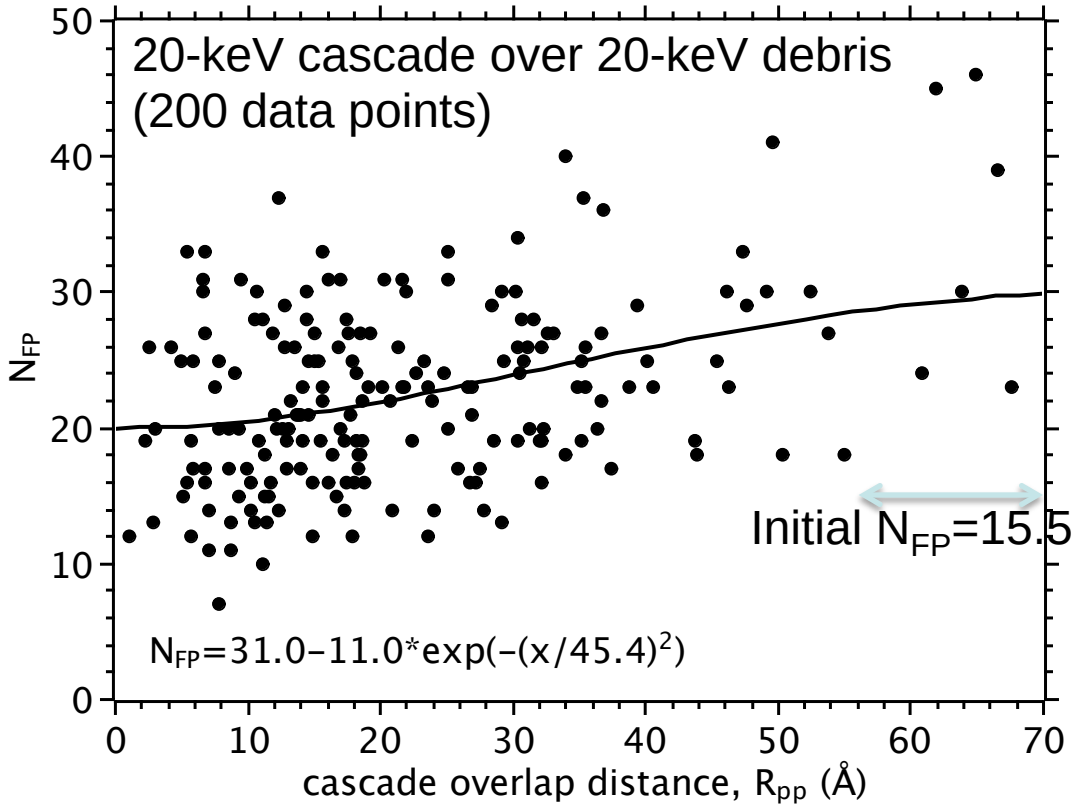


W lattice defects near the bubbles



Modeling cascade damage in "bulk" tungsten

- Under extreme neutron fluxes, cascade overlap will occur.
- Currently there are no clear methodologies on how to model cascade overlap in long-time defect evolution simulations using object kinetic Monte Carlo methods.
- We utilize molecular dynamics simulations to develop basic understanding.
- 20-keV overlapping cascades in tungsten at 1025 K performed.
- Each cascade is followed up to 20 ps.
- A reduction in N_{FP} per cascade due to overlap is observed.



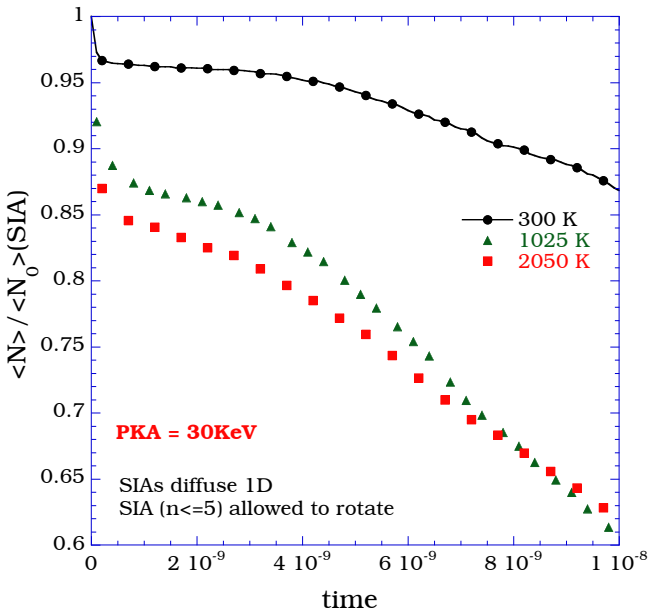
Fit constraint: $N_{FP}(\infty)$ = 2*initial N_{FP}

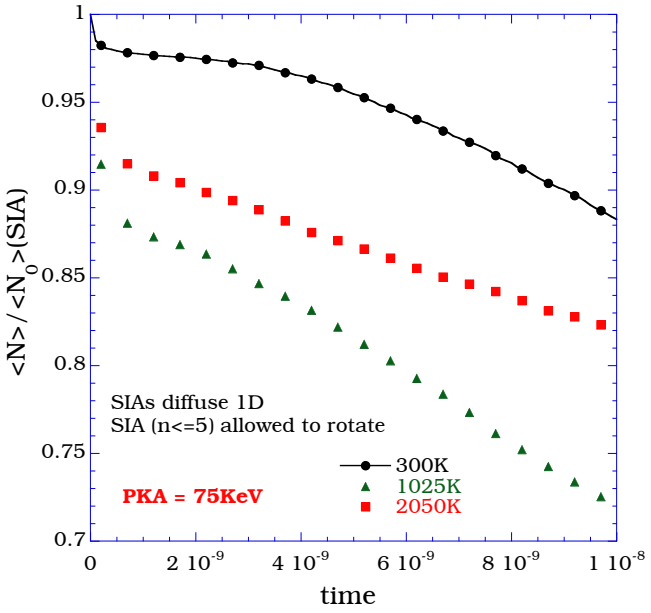
KSOME: Long-time defect evolution

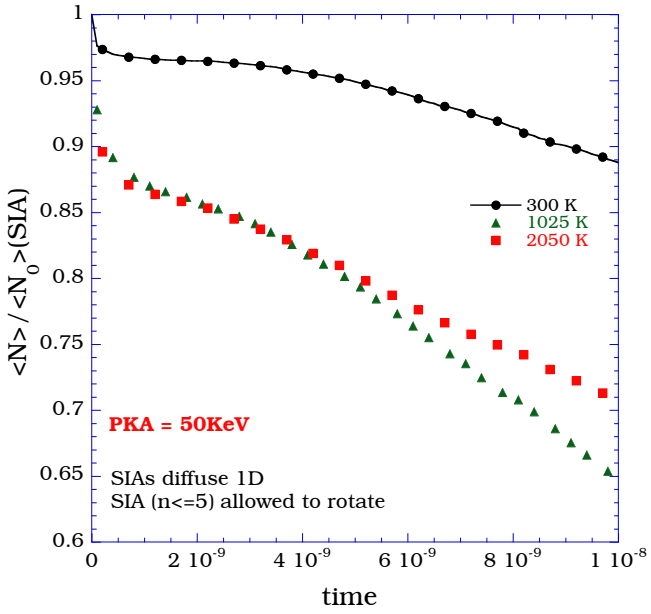
- An advanced object kinetic Monte Carlo code called KSOME (Kinetic Simulation of Microstructure Evolution) has been developed to simulate the evolution in time and space the distribution of defects in crystalline solids accumulated during neutron irradiation.
- KSOME is designed to simulate the diffusion, emission, transformation and reaction events of vacancies, interstitials, impurities and their complexes, including any number of combinations of point defects, for bcc and fcc lattices at a given temperature.
- Cascade insertion is random, based on a specified cascade production rate and allows for creation of any type of defect based on their production probability.
- Interaction of mobile defects (simple absorption) with sinks such as dislocations, grain boundaries and free surfaces.
- Defect parameters like type, size, orientation, etc. are used to identify defect diffusion, emission, reaction and transformation events between various types of defects.
- Example events:
  - → Rotation or change of direction of 1D-diffusing SIA clusters
  - → Vacancy loop transforming into a spherical cluster or void
  - → Emission can also be associated with a loop punching or trap mutation event
  - → Allows emission of multiple (size or type) defects from a single source

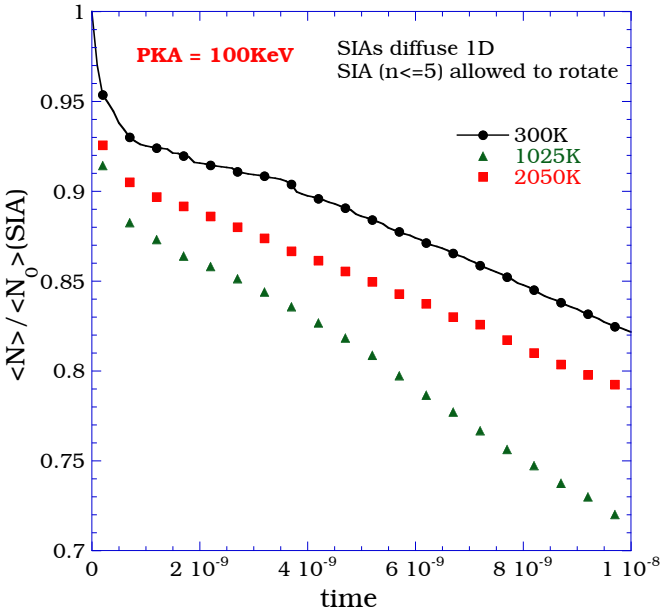
Defect evolution during cascade aging: KSOME

Effects of Temperature and PKA Energy









Vacancies: m ≥ 5 (%)

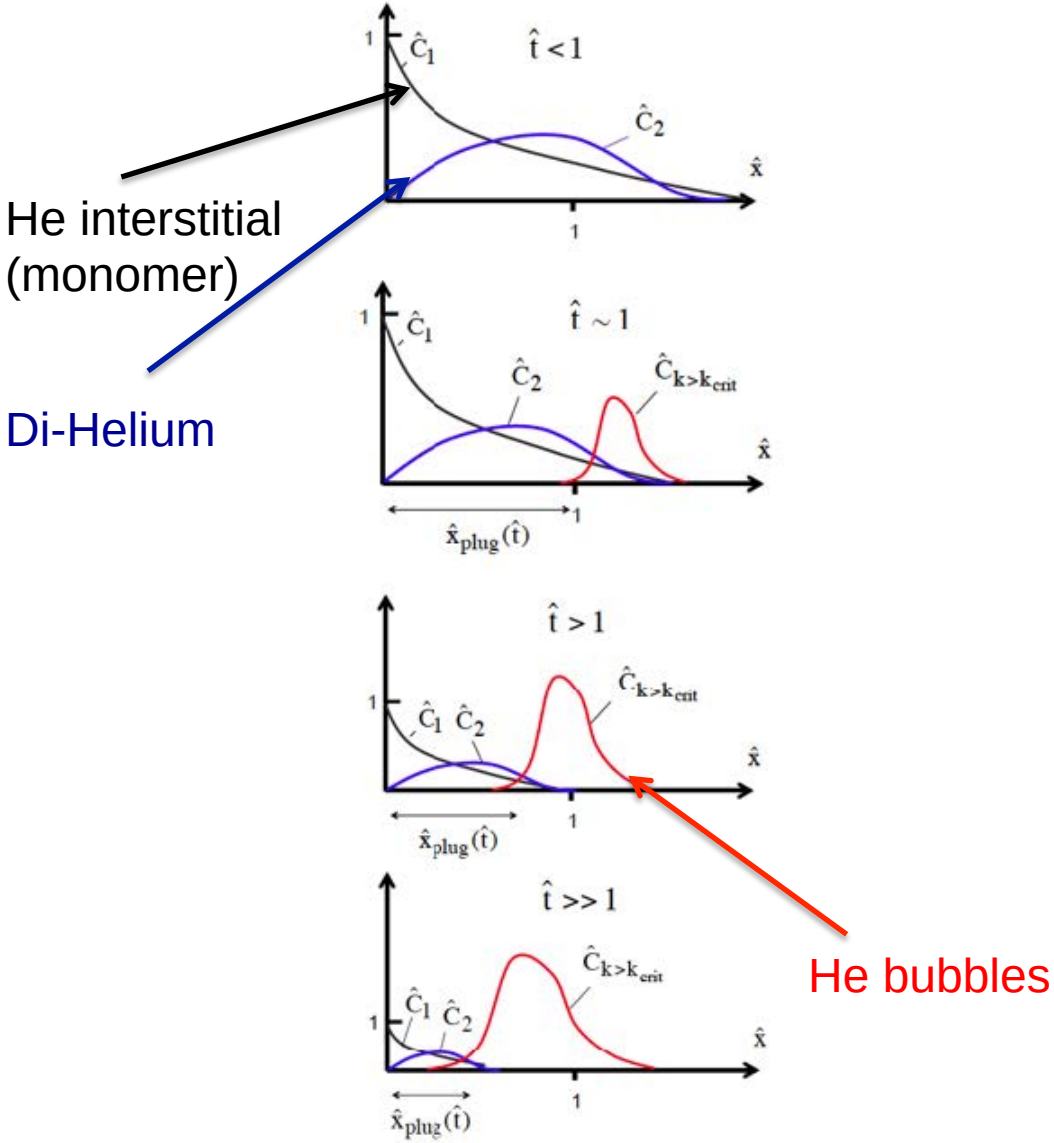
PKA	300	1025	2050
30	4	0	0
50	16	14	0
75	21	23	6
100	31	27	5

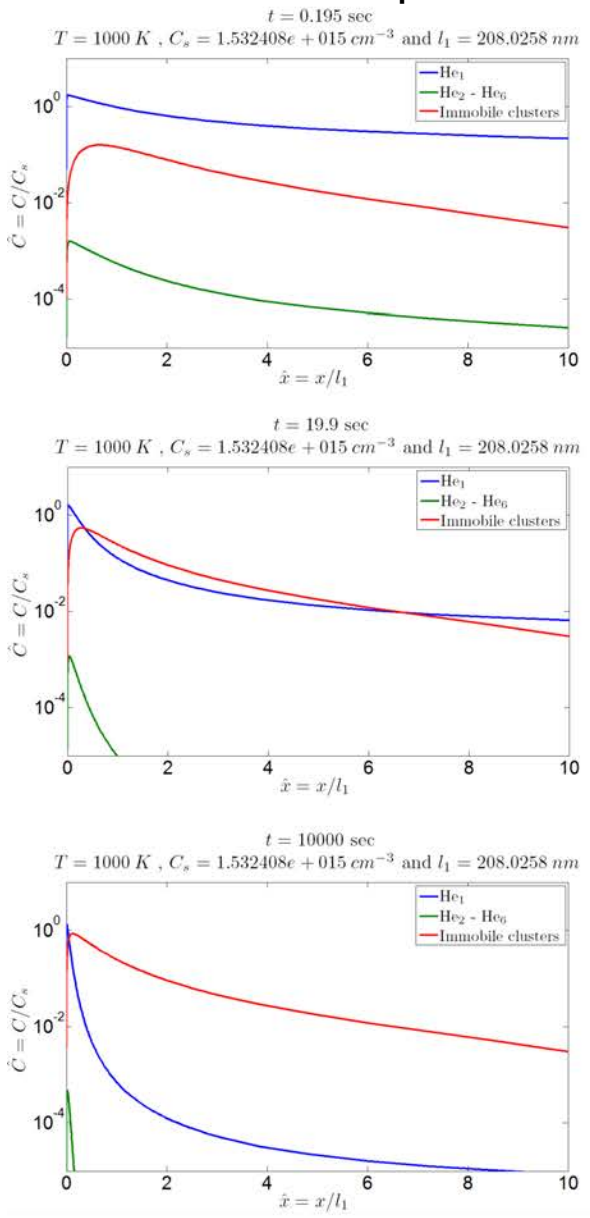
SIA: m ≥ 5 (%)

PKA	300	1025	2050
30	19	11	30
50	34	30	42
75	38	33	69
100	46	52	64

*Theoretical analysis of He clustering/bubble formation**

• Theory and detailed continuum reaction-diffusion model reveals a layer of helium bubbles (denoted as a plug) below tungsten surfaces at intermediate temperature





* Krasheninnikov, Faney and Wirth, *Nuclear Fusion* **54** (2014) 073019

Validation of simulations: Experiments at DIII-D

The 3D Monte Carlo code ERO:

- Plasma-surface interaction
- Local impurity transport

First step: benchmarking

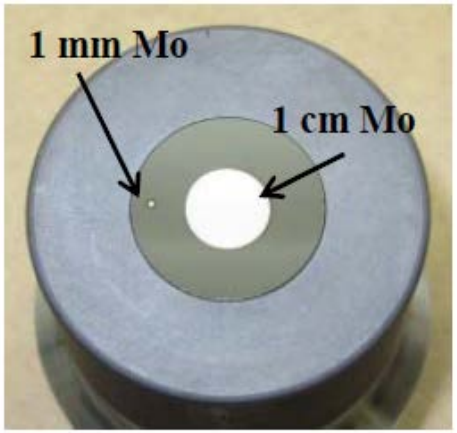
WBC/REDEP/ITMC code (J.N. Brooks)

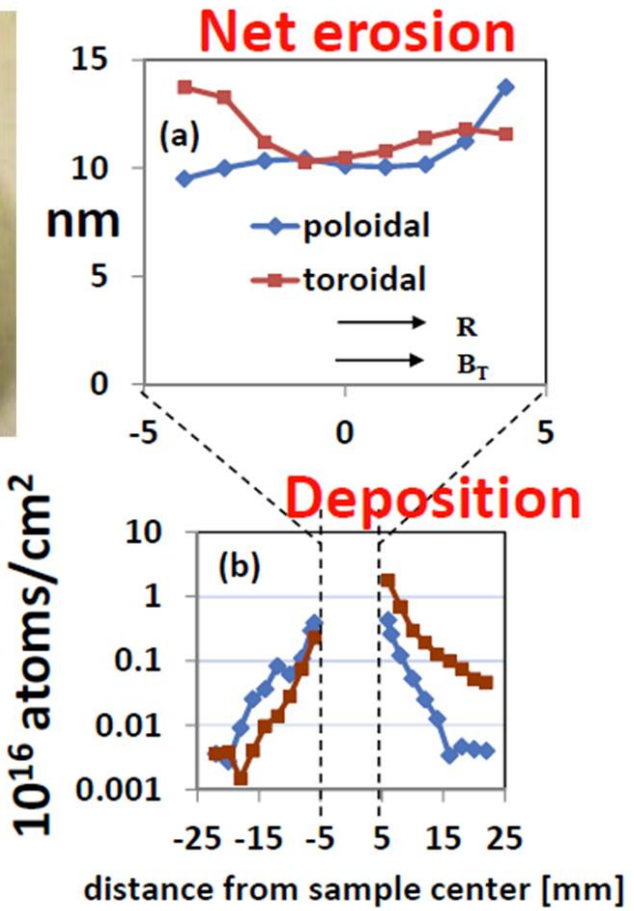
Next step:

- Analysis of new DiMES results
- Modelling of DIII-D $^{13}CH_4$ injection experiments
- Modelling of forthcoming He-W experiments

DIMES experiments:

Gross vs net erosion of Mo and W





Summary & Future Challenges

- Strong interactions within team & with SciDAC Institutes

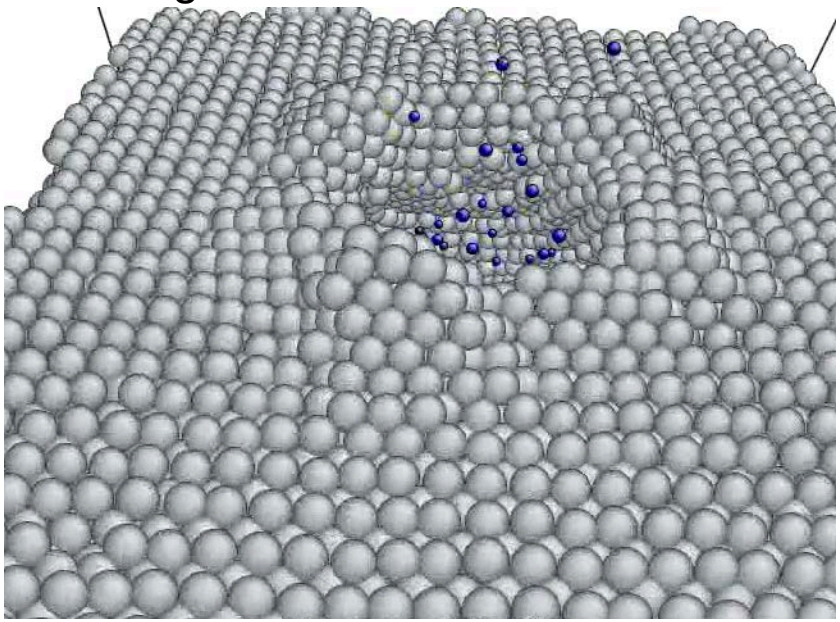
- Initial discovery science to provide mechanistic understanding of W surface dynamics under low-energy He plasma exposure & initial integration with experimental efforts
  - Characterized thermodynamics/kinetics of small He clusters
  - Discovery of interaction mechanisms of helium as small clusters serve as bubble nuclei with realistic microstructures, rate effects of helium bubble growth and coalescence
  - Quantifying defect production and aging evolution in “bulk” tungsten due to high-energy neutron irradiation
  - Development of new KMC code (kSOME) & continuum PSI simulator (Xolotl); strong engagement with Performance/Optimization, (SUPER), ADR solvers in PETSc (FASTMath), SDAV & QUEST
  - Reduced parameter models of helium bubble evolution agree well with detailed cluster dynamics simulations
  - Experimental validation available through DIII-D experiments

- Successful completion of the project (2017) will provide simulation tools to evaluate tungsten-based plasma facing component and divertor components in a burning plasma environment.

Molecular Dynamics calculations

- **'Common' MD codes: LAMMPS, SPASM**
  - **typically run on small clusters (usually because of throughput), especially for 'discovery' science**
  - **increasingly used for 10^7 atoms & beyond (provide decreased implantation rates)**
  - **limited by interatomic potentials and achievable timescales**
  - **Accelerated MD has potential to increase timescale but generally limited to specific phenomena (e.g., bubble growth) in small systems (O~10^3 atoms)**

Bursting of He bubble onto W surface



Typical MD run times, ANL Mira
- O(2×10^7 atoms), O(2×10^4 cores)

1 MD timestep, O(10^{-15} sec) requires
1 ms (10^{-3} s) wallclock time

Thus, to reach 10^4 seconds (onset of fuzz formation) requires 10^{19} MD timesteps & 10^{16} seconds **O(1 Billion years)**