Plasma Surface Interactions (PSI): Bridging from the Surface to the Micron Frontier through Leadership Class Computing

Brian D. Wirth*,#, F. Sefta, T. Faney, K. Hammond, N. Juslin, and D. Xu, on behalf of

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ORNL	Brian D Wirth	David E. Bernholdt, Jay Jay Billings, John Canik, Jeremy Meredith (SDAV), Philip C. Roth (SUPER), Roger Stoller, Stanislav Golubov
PNNL	Rick Kurtz	Giridhar Nandipati, Kenny Roche
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UIUC	David Ruzic	Davide Curreli, Kyle Lindquist
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Rockville, MD

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A word about us: we're just getting started

SciDAC Project kick-off meeting

Plasma Surface Interactions: Bridging from the Surface to the Micron Frontier through Leadership Class Computing

Meeting objective: Define specific work tasks and deliverables for each project team within the first year. Build synergistic interactions amongst team members and projects.

Argonne National Laboratory, Building 240, Room 1404-5

Time	Wednesday, 5 Sept	Thursday, 6 Sept	Friday, 7 Sept
8:30	Welcome, Introduction and Objectives, (B. Wirth, D. Bernholdt and T. Tautges)	Welcome, Introduction and Objectives, (B. Wirth, D. Bernholdt and T. Tautges)	Welcome, Introduction and Objectives, (B. Wirth, D. Bernholdt and T. Tautges)
8:45	Introduction to PSI Challenges (B. Wirth, S. Krasheninnikov)	Applied Math/Numerical Methods/Computer Science Challenges (D. Bernholdt, B. Smith, T. Faney)	Discussion of Interactions, Tasks and Milestones (all)
10:15	Break	Break	Break
10:30	Edge/Scrape off Layer Modeling (X. Tang, J. Canik)	Uncertainty Quantification, Performance Issues & Visualization capabilities and needs (D. Higdon, P. Roth, K. Roche, J. Ahrens, J. Meredith)	Summary of Tasks and Milestones (all)
12:15	Lunch, on own	Lunch, on own	Adjourn
1:30	MD/AMD & Interatomic Potentials for W-He-H (B. Uberuaga, N. Juslin)	Paraspace and XOLOTL – PSI Code development approach (D. Xu, J.J. Billings, T. Tautges)	
3:15	Break	Break	
3:45	KMC/Hierarchical Multiscale Modeling Approaches (R. Kurtz, D. Maroudas, R.E. Stoller)	Experimental validation targets (D. Ruzic, V. Chan)	
5:30	Summary discussion	Summary discussion	
6:00	Adjourn	Adjourn	

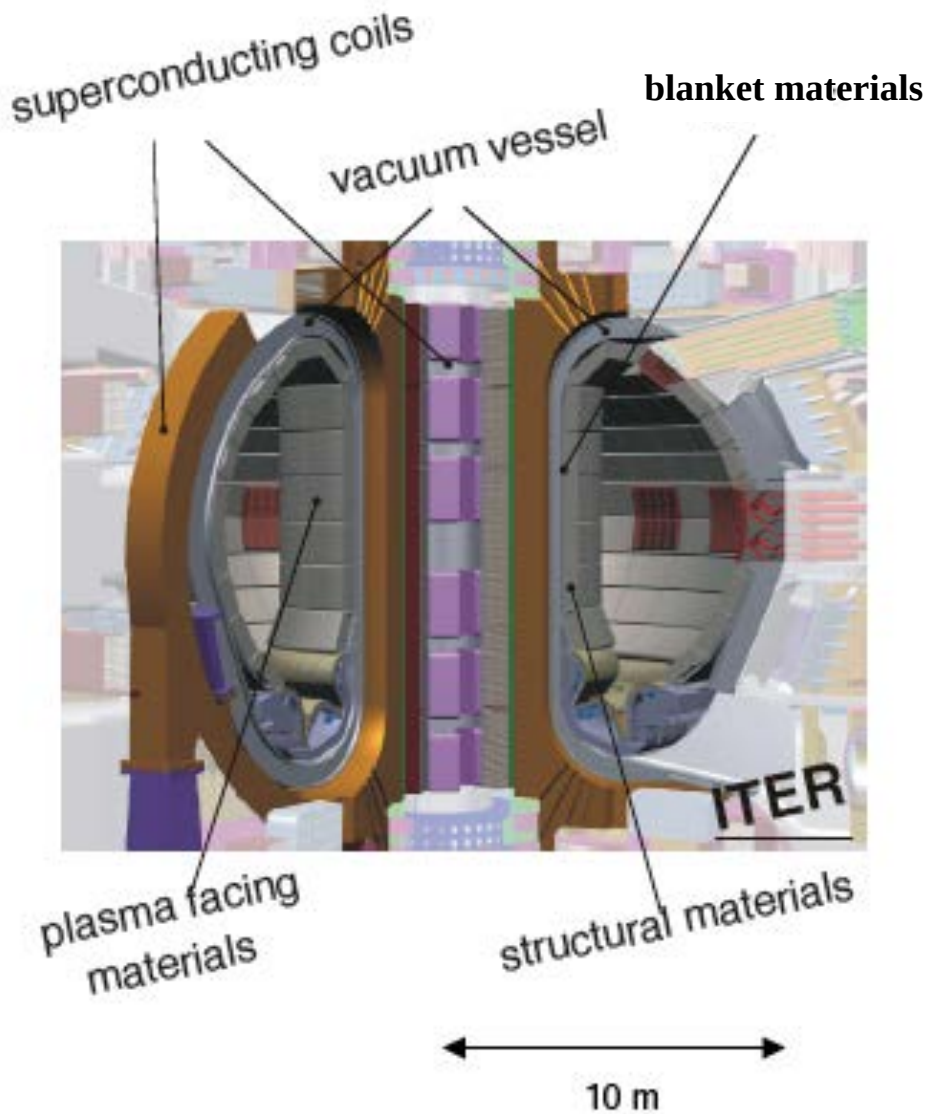
Identify tasks/milestones, experimental validation targets (specific experiments, conditions) for initial 12-18 months of effort

Complement on-going activities and utilize key resources

Focus on materials aspects of plasma surface interactions, but with small efforts at plasma edge/ scrape off layer & bulk materials to identify future code-coupling

*Materials issues in Magnetic Fusion Energy (ITER/DEMO)**

- **Magnetic fusion energy presents many materials challenges, including:**
  - **High thermal heat fluxes**
  - **Erosion/Sputtering/blistering of plasma facing components**
  - **Radiation damage**
  - **Low induced radioactivity**
  - **Chemical compatibility**
  - **Joining/Welding**



NAE Grand Challenge for Engineering:
2. Provide energy from fusion

***Ref: H. Bolt, Max-Planck Institute for Plasma Physics, Garching, Germany**

*Plasma Facing Components/Materials (ITER)**

Key issues

- erosion lifetime and plasma compatibility
- tritium inventory
- thermal transients
- **He blistering**
- heat removal:
- fabrication technology:
- neutron damage:

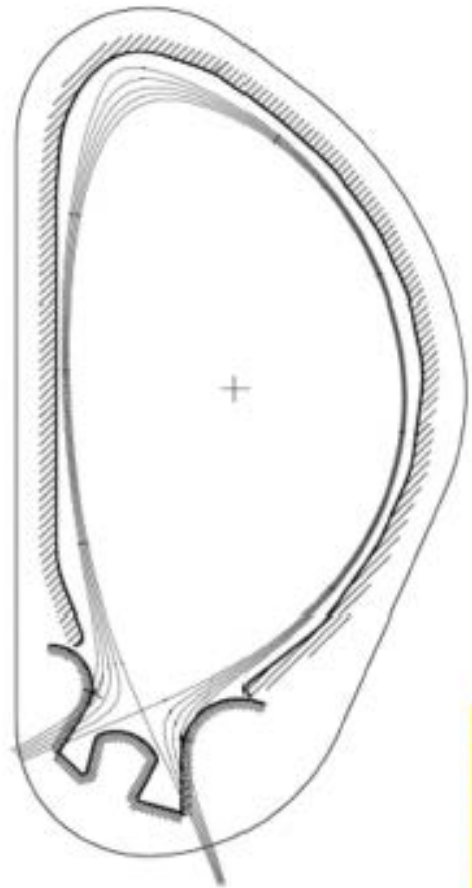
Leading candidate materials

PFC and Divertor:

- **Be, W, (C ?)**

Structural components:

- **Fe-Cr steels, V-Cr-Ti, SiC**



bulk plasma:

impurity tolerance

W < 2 10^{-5}, reactor < 10^{-4}

Be, C: 10^{-2}

first wall:

modest flux of high energy neutral particles (100s eV),

low energy ions

divertor target:

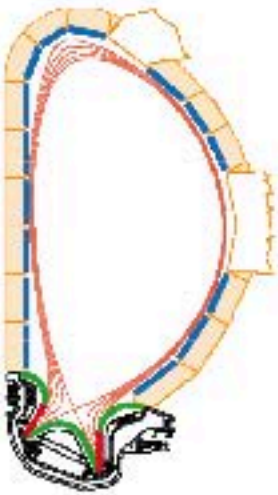
high heat flux 10 (20) MW/m^2

transient heat loads:

e.g. ELMs, disruptions

***Ref: H. Bolt, Max-Planck Institute for Plasma Physics, Garching, Germany**

*PFC Materials: Surface chemistry evolves as well**



ITER

- First wall on ITER
  - → carbon (?) 55 m^2
  - → tungsten 140 m^2
  - → beryllium 690 m^2
- DEMO first wall / divertor
  - → oxidation-resistant W alloys (e.g. W—Si—Cr)
- Variable local conditions (temperature, fluence, species…)
- Erosion and redeposition, impurities:
  - → mixed phases (e.g. oxides, tungsten – beryllium alloys)
- Layers on metals influence:
  - → hydrogen inventory: reaction, diffusion, desorption
  - → physical and chemical processes: sputtering, reactions
- Goal: qualitative and quantitative description of fundamental processes
  - → formation and erosion of multi-component layers
  - → influence of layers on hydrogen inventory

→ **Include surface reactions in global integrated PWI model**

Ref: * C. Linsemeier, PSI-19 Invited Presentation (2010).

*Complex, interlinked PSI phenomena**

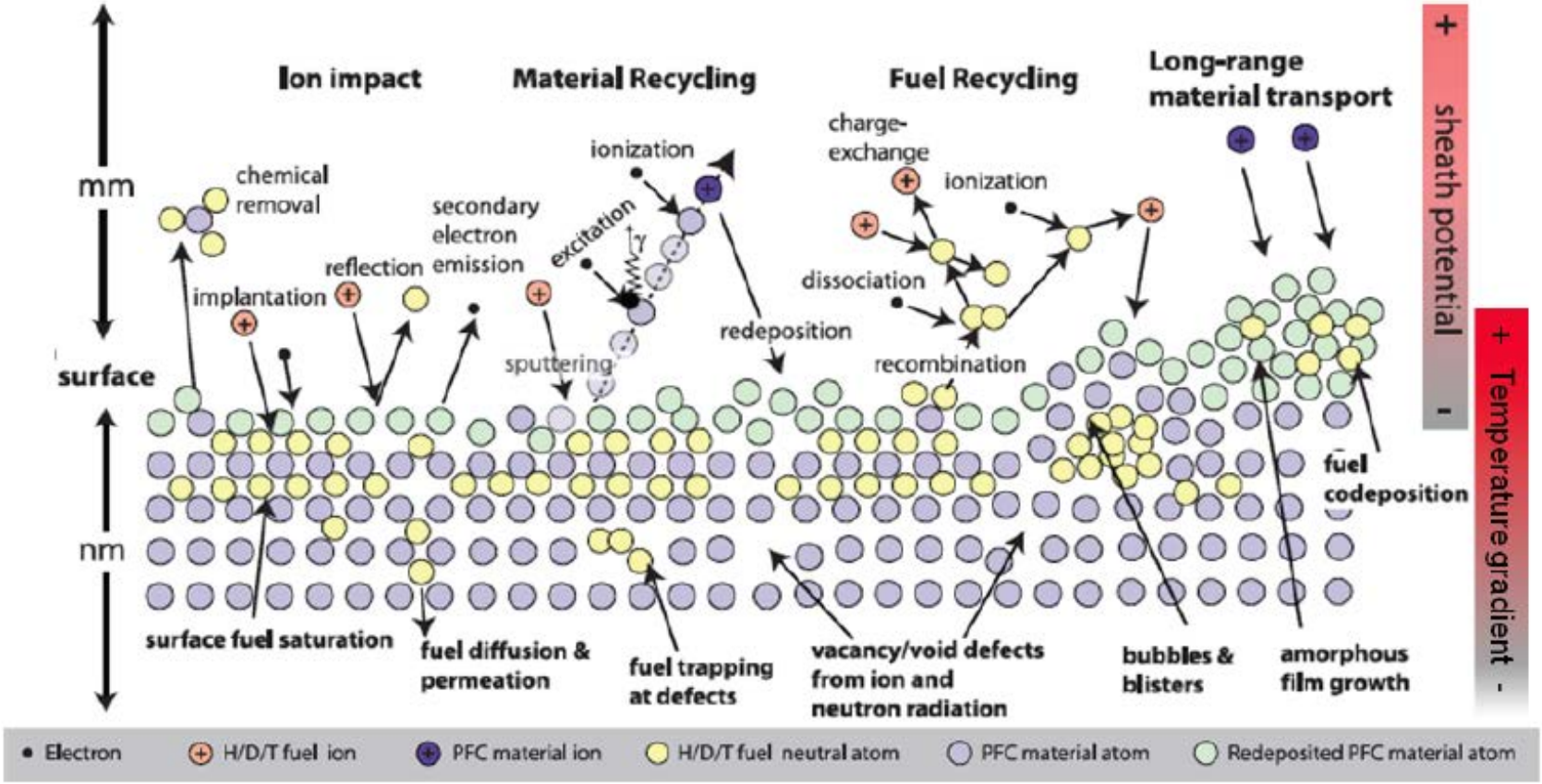


Figure of merit:
Incident plasma ion flux near divertor strikepoint: 10^{24} $m^{-2}s^{-1}$

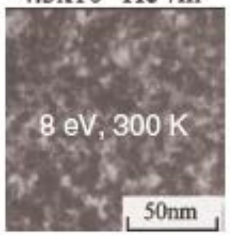
Steady-state sputtering yield O (10^{-4}) on surface monolayer (10^{19} atoms/m^2) results in sputtering of every atom every 0.1 sec -> every atom sputter >10^8 times/year

* Wirth, Nordlund, Whyte, and Xu, *Materials Research Society Bulletin* **36** (2011) 216-222

W Surface dynamics under combined thermal/particle fluxes

T < 700 K

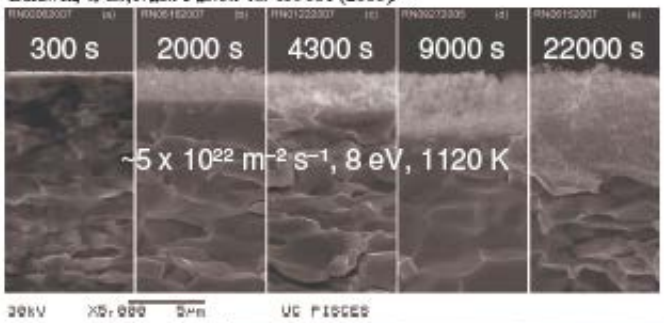
4.3x10^{19}He^{+}/m^{2}



H. Iwakiri, *et al.*, *J. Nucl. Mater.* 283–287: 1134–1138 (2000).

non-specific damage

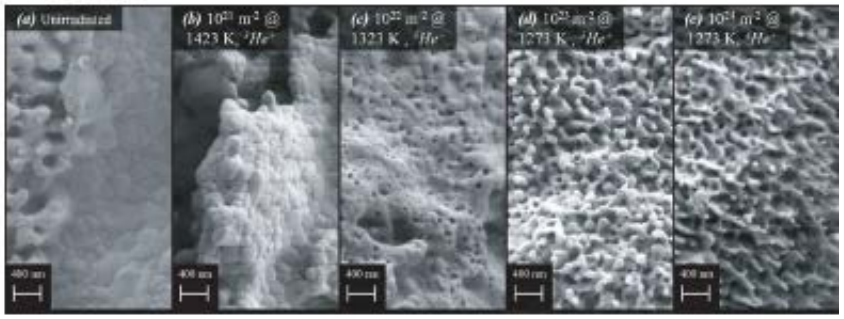
Baldwin, *et al.*, *Nucl. Fusion* 48: 035001 (2008).



900 K < T < 1900 K

fuzz / coral

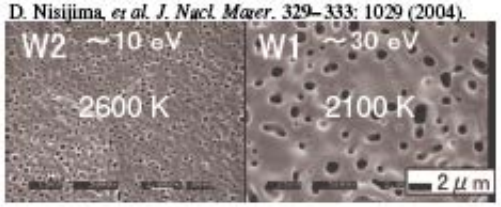
S. J. Zenobia and G. L. Kulcinski. *Phys. Scr.* T138: 014049 (2009).

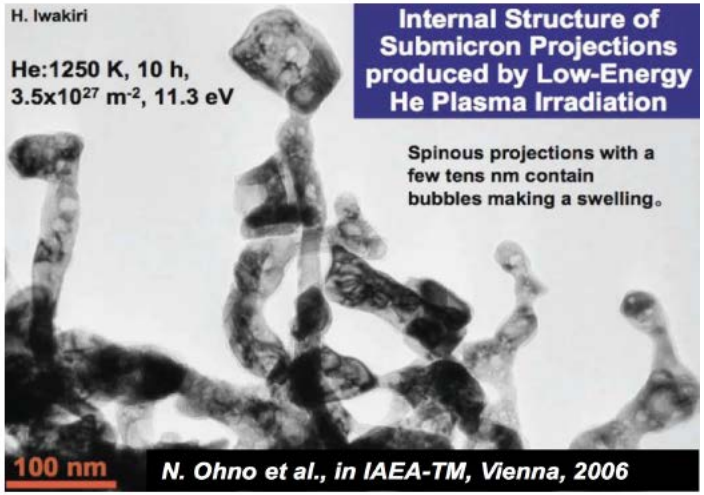


T > 2000 K

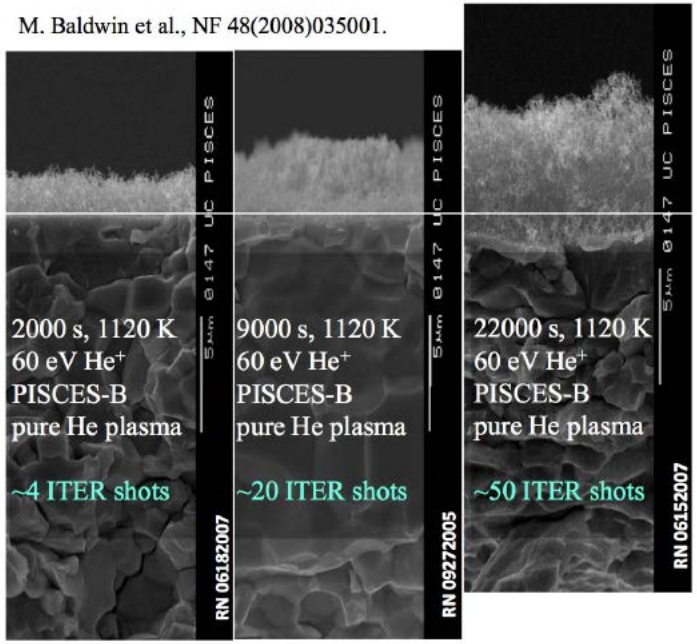
holes

D. Nisijima, *et al. J. Nucl. Mater.* 329–333: 1029 (2004).

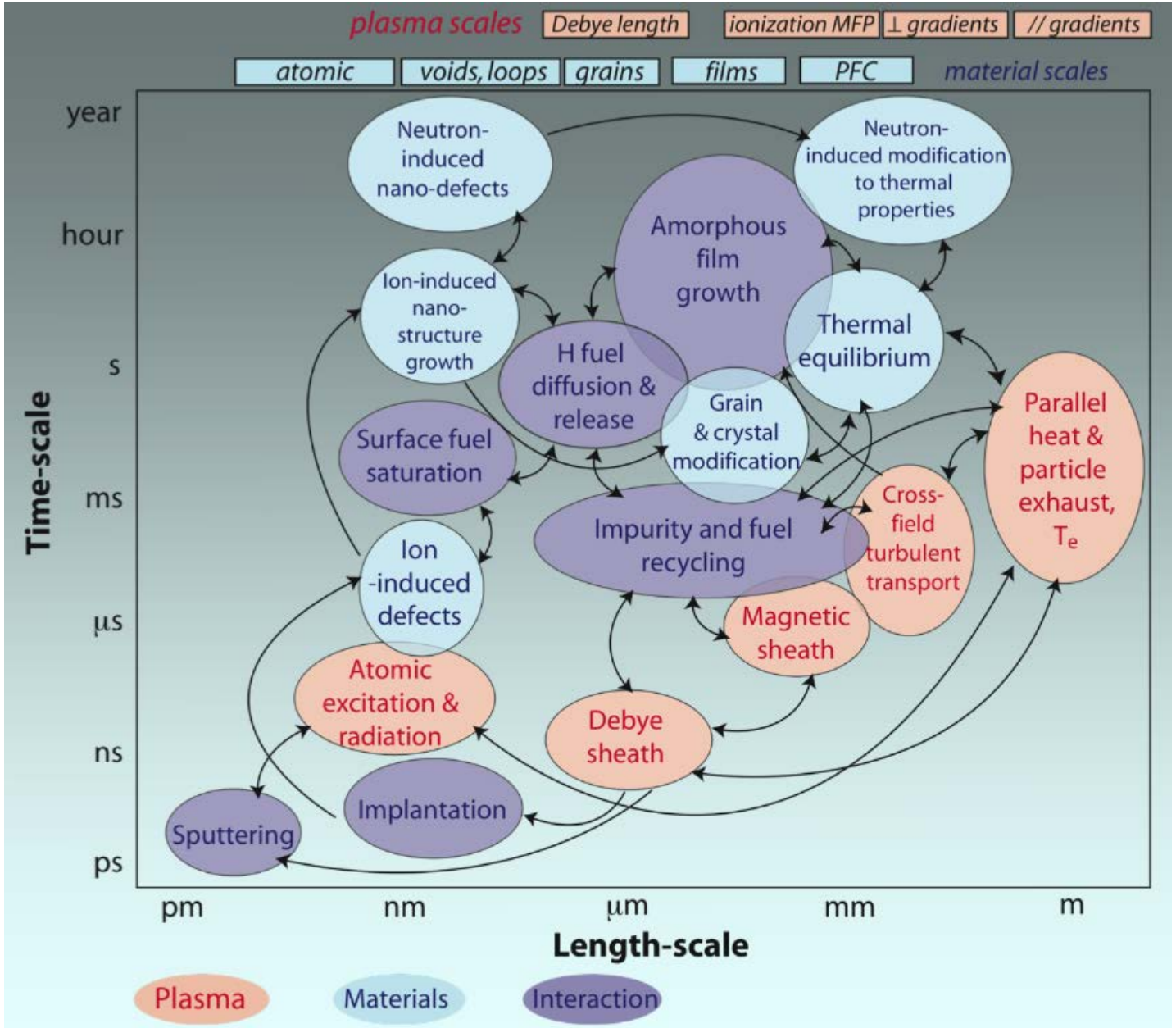




M. Baldwin et al., NF 48(2008)035001.

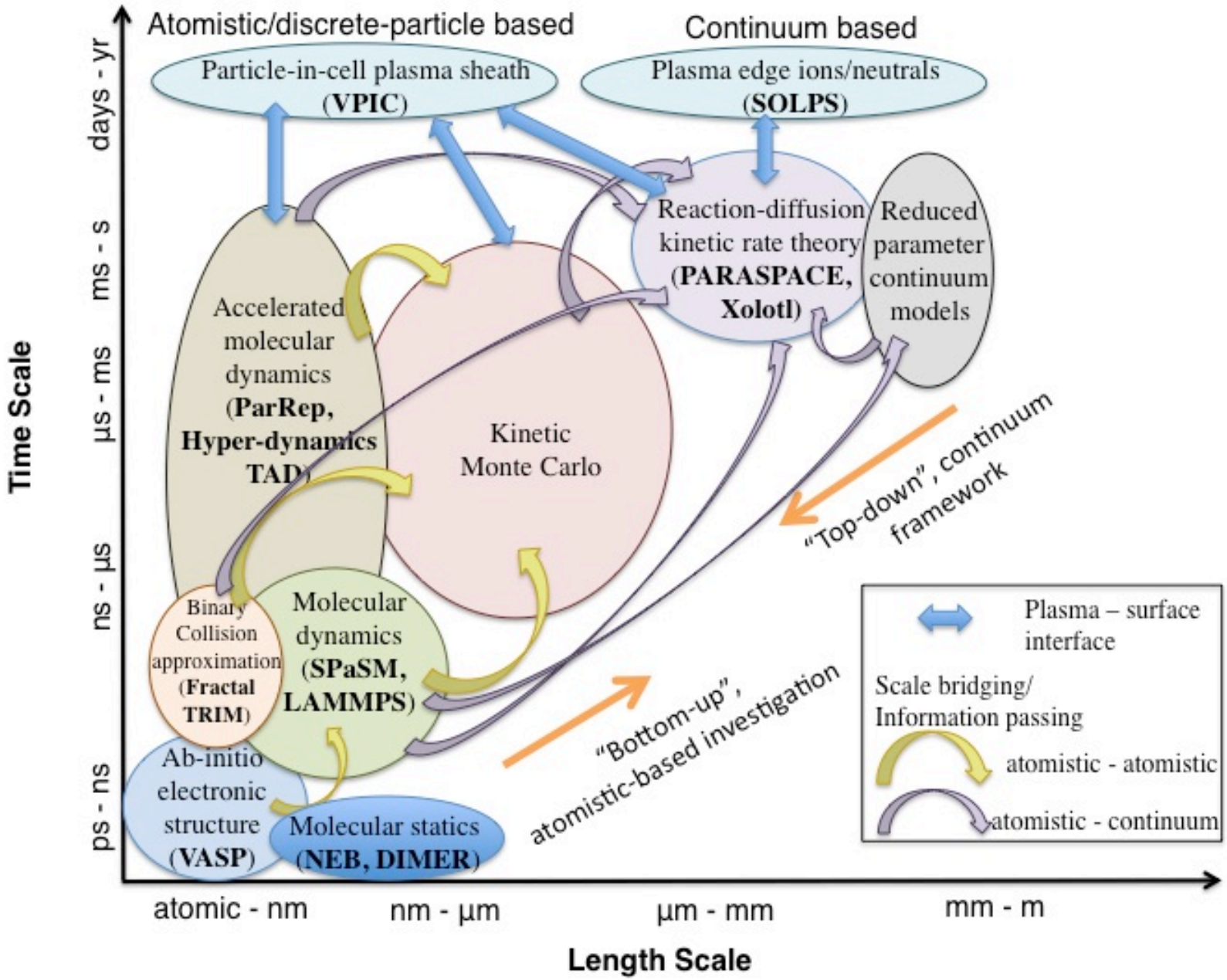


*Multiscale, interlinked Plasma-Surface Interaction phenomena**



* Wirth, Nordlund, Whyte, and Xu, *Materials Research Society Bulletin* **36** (2011) 216-222

Multiscale modeling approach for SciDac



Key Computational Science Challenges

- Scalable algebraic and geometric multigrid methods for reaction-diffusion type problems, differential variational inequality (DVI) solvers, implicit-explicit (IMEX) ordinary differential equation (ODE) integrators, and mesh coupling algorithms and software from the Frameworks, Algorithms, and Scalable Technologies for Mathematics (FASTMath)
- Forward uncertainty propagation, inverse modeling and parameter estimation, linking information and uncertainties across scales, and information about model inadequacies from the Quantification of Uncertainty in Extreme Scale Computations (QUEST) Institute
- Dynamic performance data collection, abstractions and tools for performance portability, and resilience techniques from the Institute for Sustained Performance, Energy and Resilience (SUPER)
- Multivariate analysis, feature identification, temporal analysis, and data formats and models from the Scalable Data-management, Analysis and Visualization (SDAV) Institute

Connection to SciDAC Institutes

- **FASTMath - Frameworks, Algorithms and Scalable Technologies for Mathematics**
  - **Tim Tautges (ANL), Barry Smith (ANL)**
- **QUEST - Quantification of Uncertainty in Extreme Scale Computations**
  - **David Higdon (LANL)**
- **SUPER - Institute for Sustained Performance, Energy and Resilience**
  - **Phil Roth (ORNL), *Ken Roche (PNNL)***
- **SDAV - Scalable Data Management, Analysis, and Visualization**
  - **Jim Ahrens (LANL), Jeremy Meredith (ORNL), Chris Sewell (LANL)**

Computing Challenges

Existing Codes (AMDF, LAMMPS, VPIC, VASP)

- **Performance and scalability**
- **Uncertainty quantification**
- **Analysis and visualization for understanding**

Coupling existing codes and Xolotl-PSI (multiscale integration)

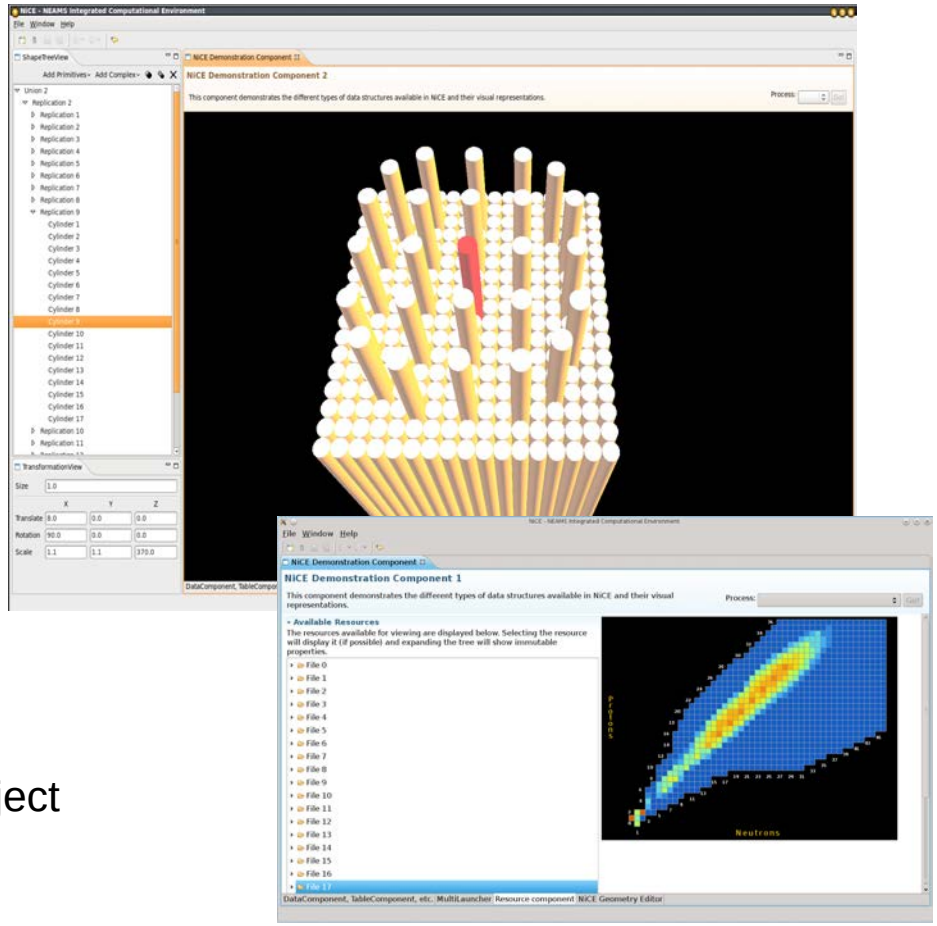
New Code (Xolotl-PSI)

- **A rare opportunity to build a major simulation code from scratch**
- **"Future-proof" architecture and design**
  - **<u>Integration</u> of performance, UQ, analysis considerations**
  - **Anticipate fault tolerance needs**
- **Suitable for current and future computer architectures**
  - **Multicore, multicore +GPU, Intel Xeon Phi (MIC), etc.**

Using XOLOTL-PSI 'NiCEly'

The NEAMS Integrated Computational Environment (NiCE) will help with all of those difficult chores for non-expert users…

- Getting code into new software systems
- Creating applications from new software systems
- Managing inputs, geometry, materials, and meshing
- Job launch and monitoring
- Data analysis and visualization
- "Asset" management



http://www.sourceforge.net/projects/niceproject

Key Materials Physics Questions

• What physical parameters control the time dependent evolution of the near-surface morphology and composition of the re-deposition layer (e.g., is this spatial re-deposition zone ever in a steady, or quasi-equilibrium, state?) – key phenomena to model include recycling, surface morphology, gas bubble, precipitate and second phase domains (including porosity), and gas fueling/recycling

• What are the effects of high-energy neutron damage on mediating, or exacerbating, near-surface defect evolution and tritium species permeation and retention?

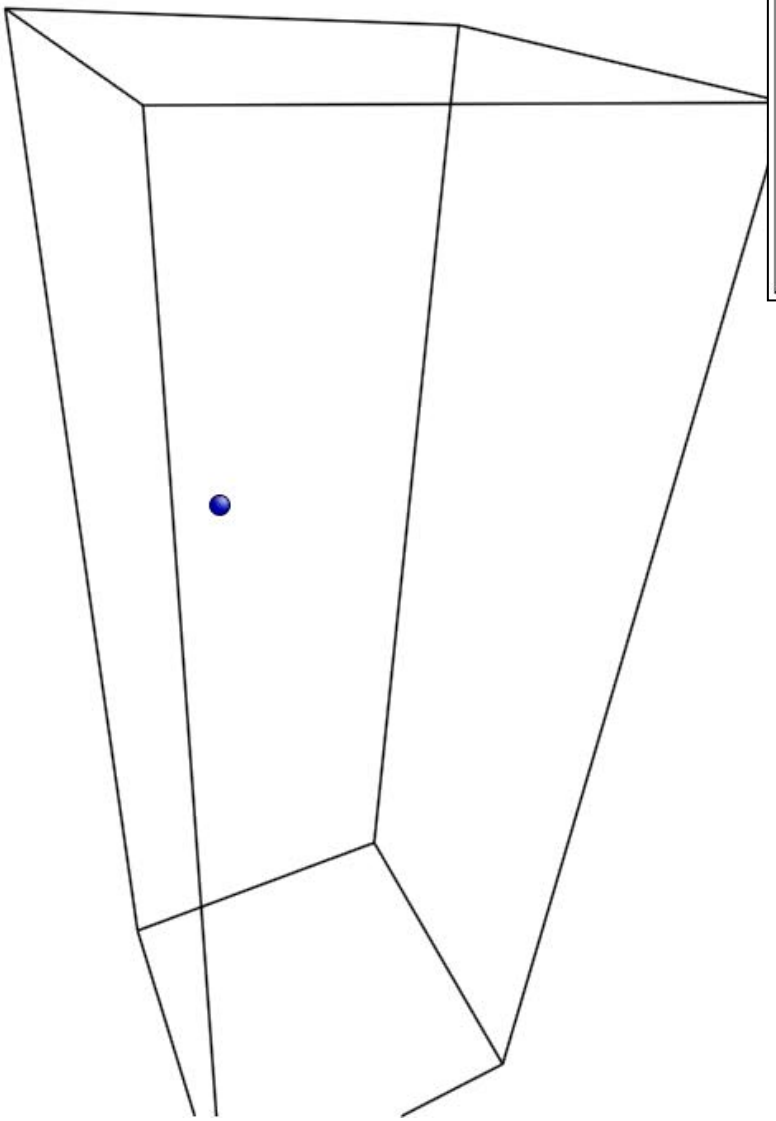
• What is the impact of dilute impurities (O, Be, …) on surface morphology evolution and plasma contamination and how does mixed material transport in tokamaks impact erosion and impurity generation?

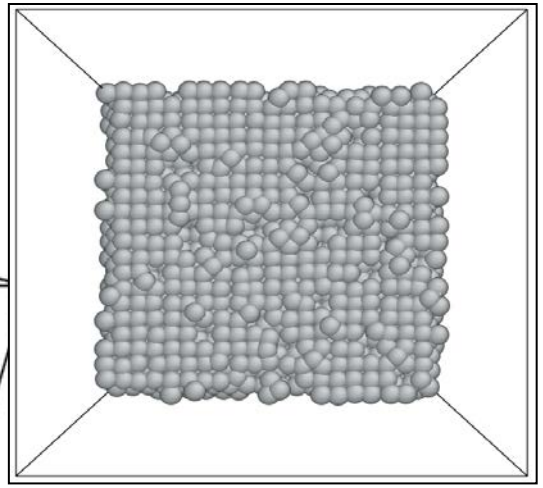
• How does the evolving bulk microstructure impact the thermal properties, and thereby feedback into PFC evolution by modifying the resulting temperature profiles?

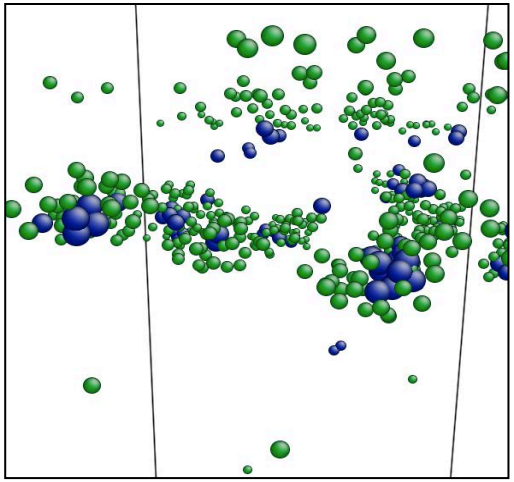
Preliminary simulation with 90%H, 10%He at 1200K

- H
- He

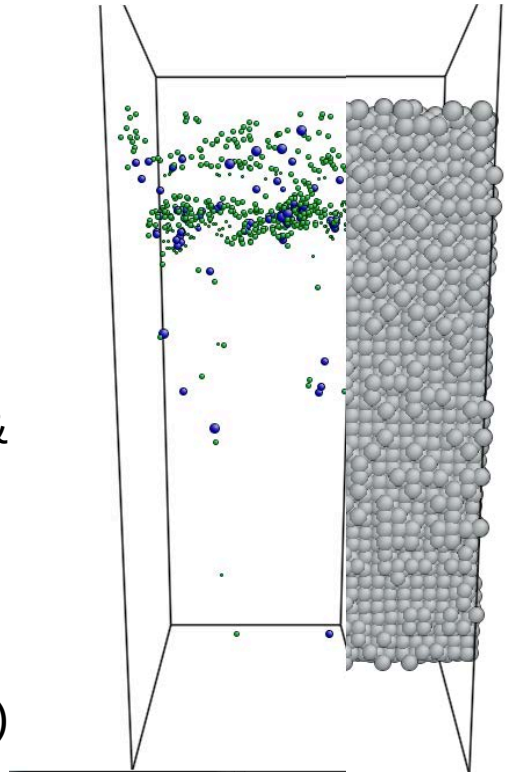
H,He introduced 1-2 nm below surface every 10 ps





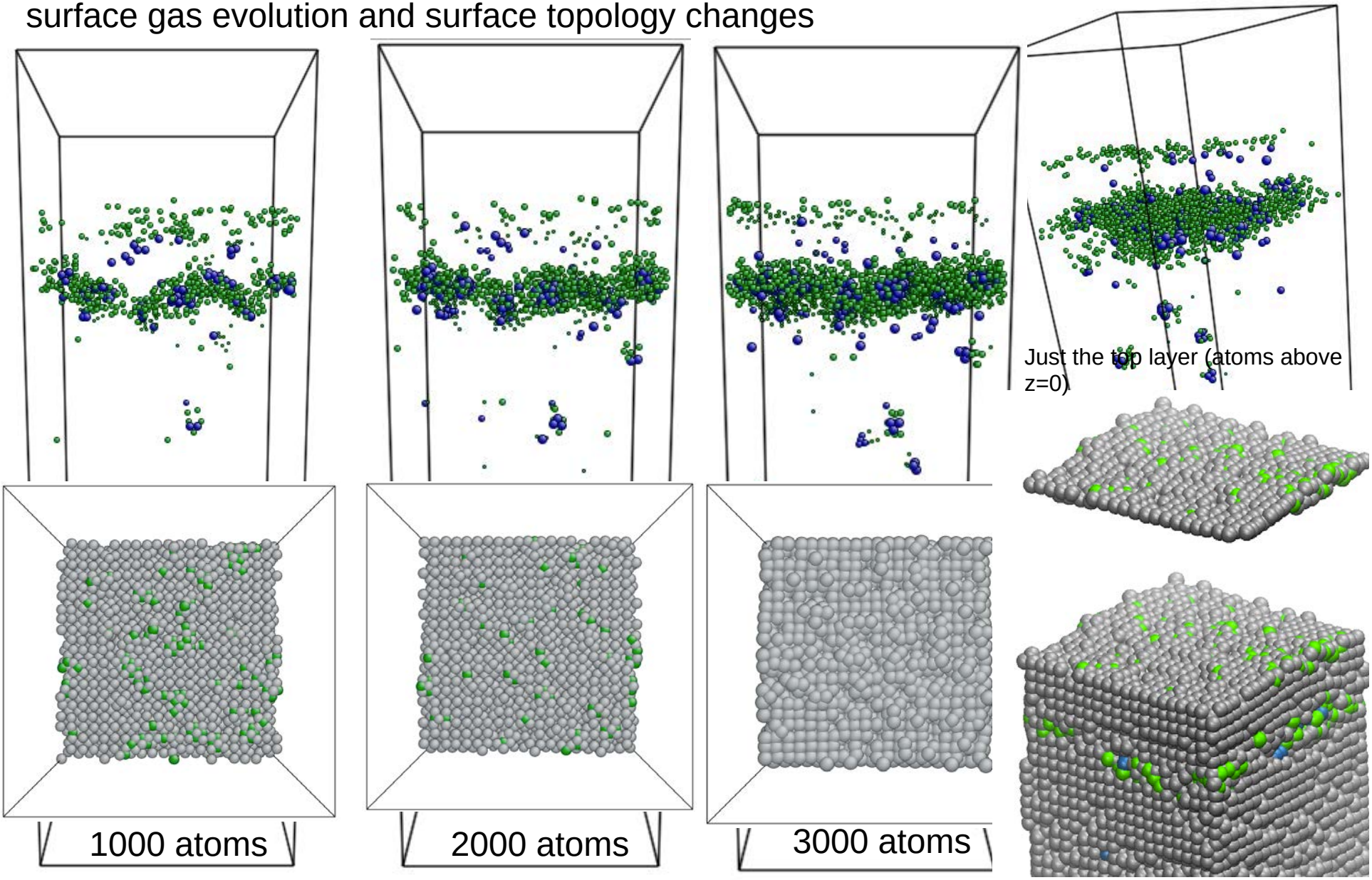


- Up to 800 implanted ions
- Significant He/H clustering
- High level of H retention (~68%) & surface saturated layers
- Increased He retention (~90% versus 68% w/o H)



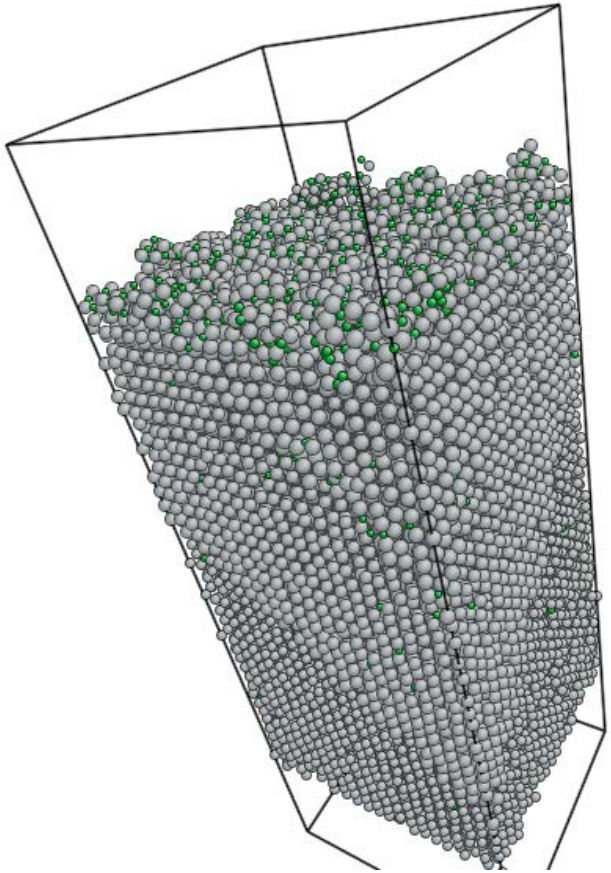
He-H Implanted in Tungsten

Mixed (90% H, 10% He) plasma exposure conditions at 1200 K, showing rapid sub-surface gas evolution and surface topology changes

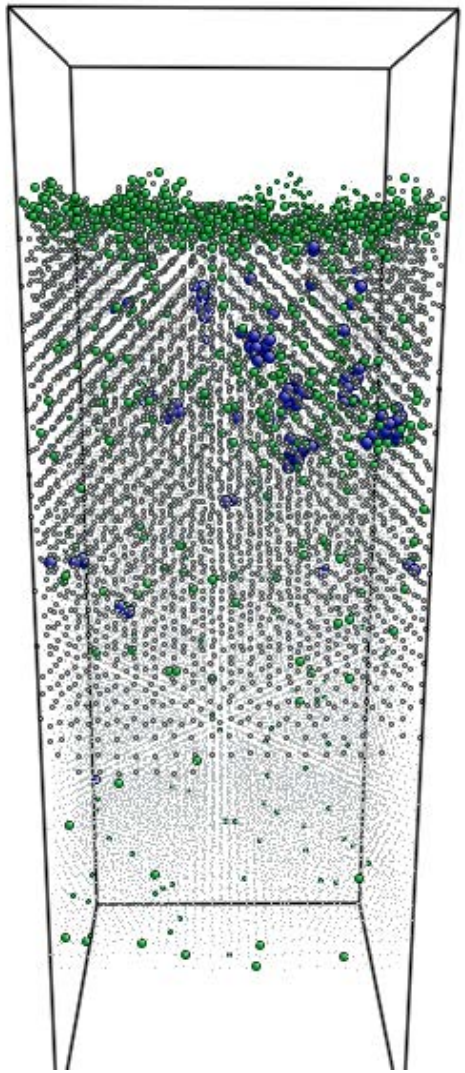


He-H Implanted in Tungsten

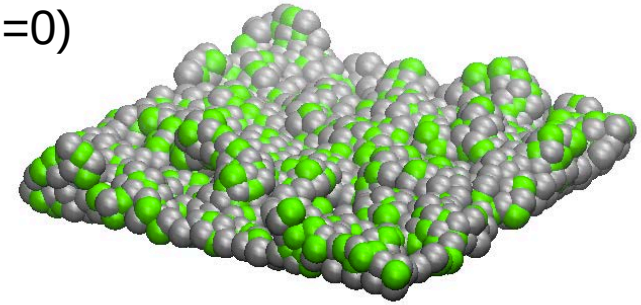
Mixed (90% H, 10% He) plasma exposure conditions at 2000 K, showing rapid sub-surface gas evolution and surface topology changes

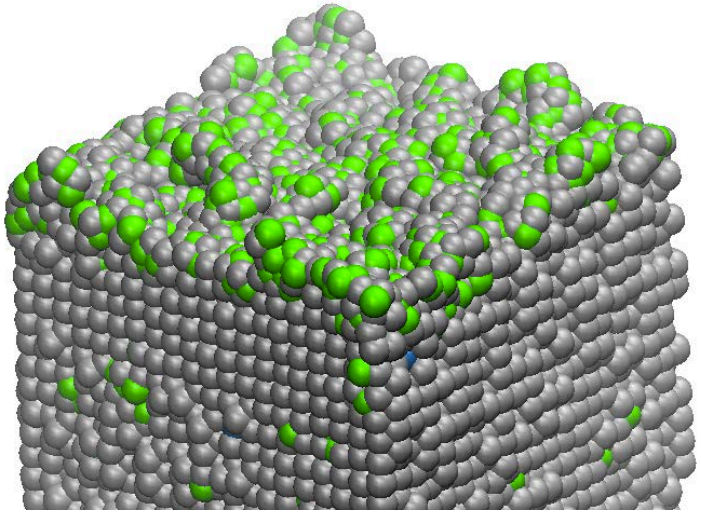


2000 atoms



Just the top layer (atoms above z=0)

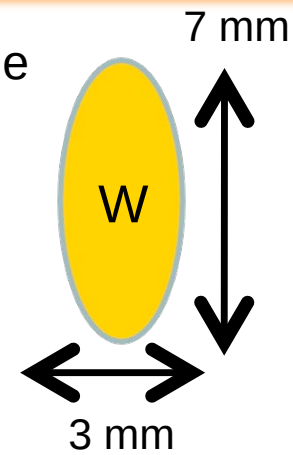


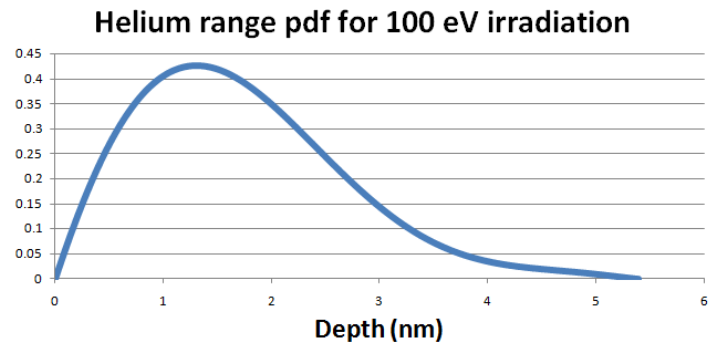


Continuum model: Low energy He implantation of W

Typical experiments: 100-500 eV He

E(He) < Sputtering Threshold Energy (~500 eV)





Coupled, 1-dimensional reaction-diffusion model:

$$\frac{\partial C_i}{\partial t}(x,t) = D_i \frac{\partial^2 C_i}{\partial x^2}(x,t) + P_i(x) - \textit{Loss at sinks} + \textit{Reaction} + \textit{Dissociation}$$

Species considered are Helium, vacancies, interstitials and their clusters, denoted by $He_x V_y I_z$, which lead to large #'s of coupled ODEs after discretization

$$M(x,t)u_t(x,t) = d(u,x,t) + r(u,x,t)$$

$$r_{(I_n)} = \sqrt{\frac{nV_a}{\pi b}} \qquad r_{(V_n)} = n^{1/3} r_a$$

Rates described by standard reaction rate theory:

C1+C2 → C3

$$R_{+,1,2} = k_{+,1,2}\,[C1]\,[C2]; \quad k_{+,1,2} = 4\pi\,(r_1 + r_2)\,(D_1 + D_2)$$

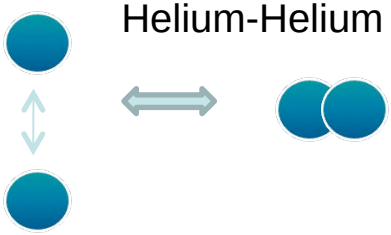
$$D = D_0 \exp(-E_m / k_B T)$$

C3 → C1+C2

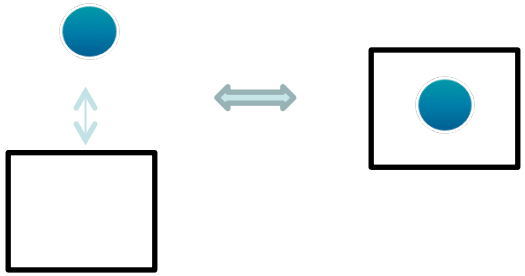
$$R_- = k_-[C3]; \quad k_- = k_{+,1,2} C_0 \exp\left(-E_{b,1in3} / k_B T\right)$$

Low energy He implantation of W

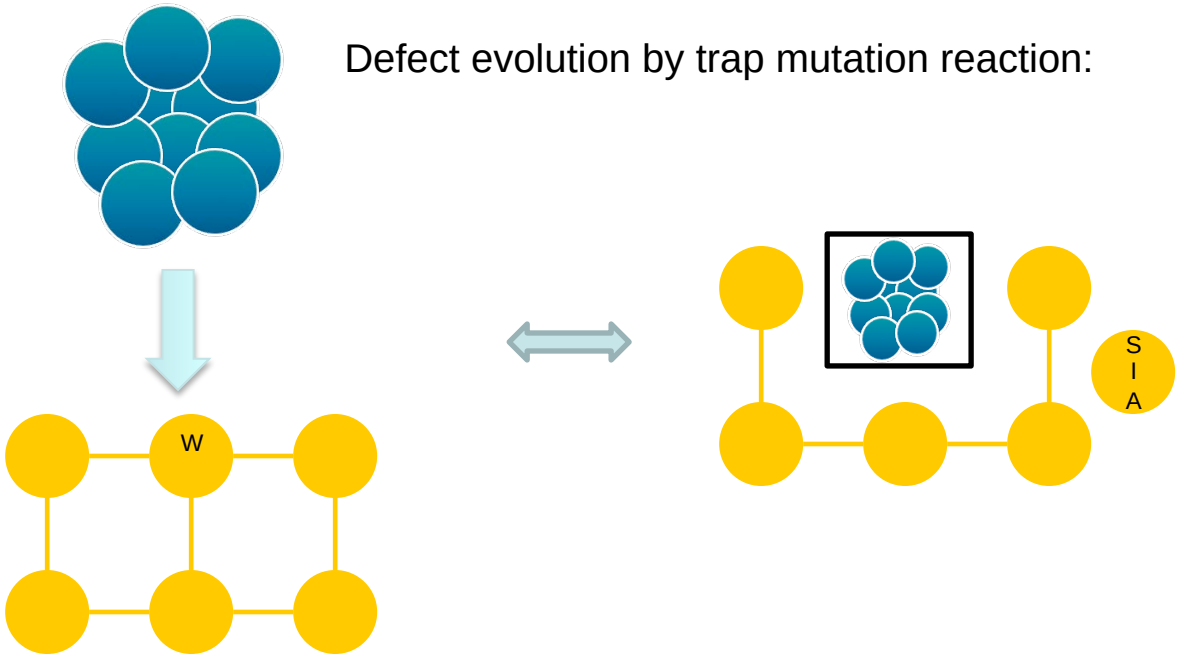
Helium-Helium Interactions



Helium – Vacancy Interactions

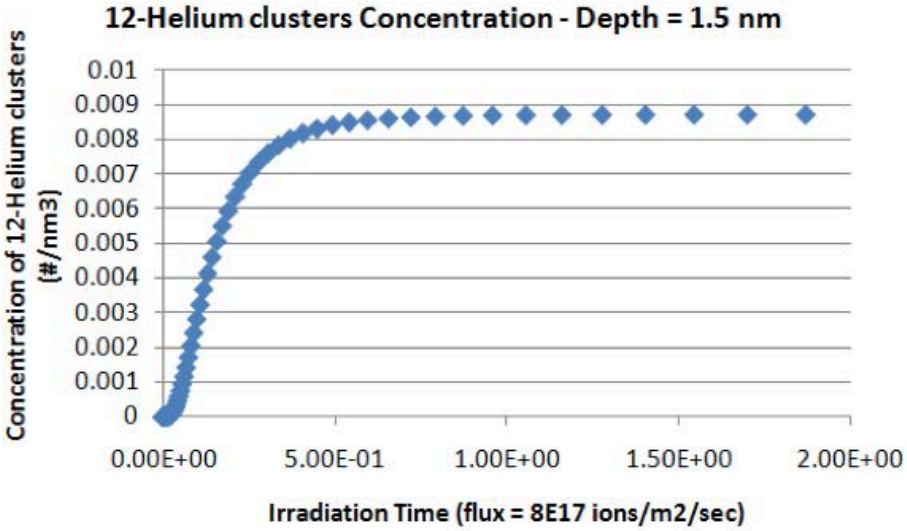


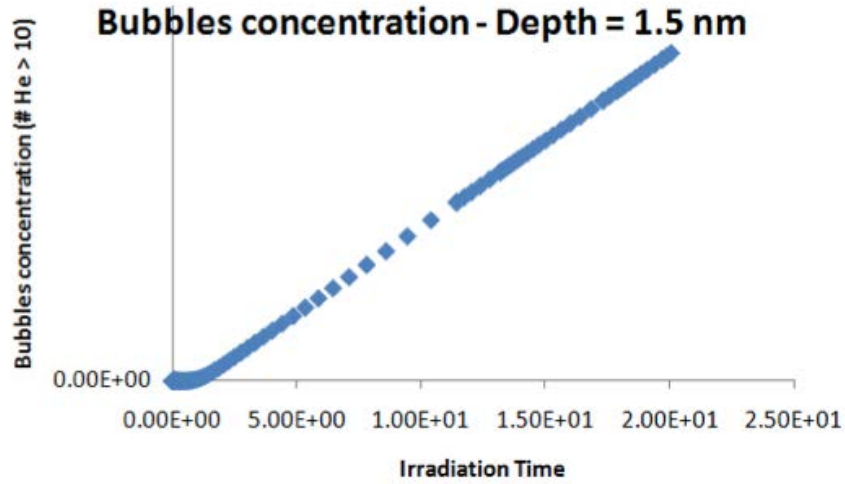
Defect evolution by trap mutation reaction:



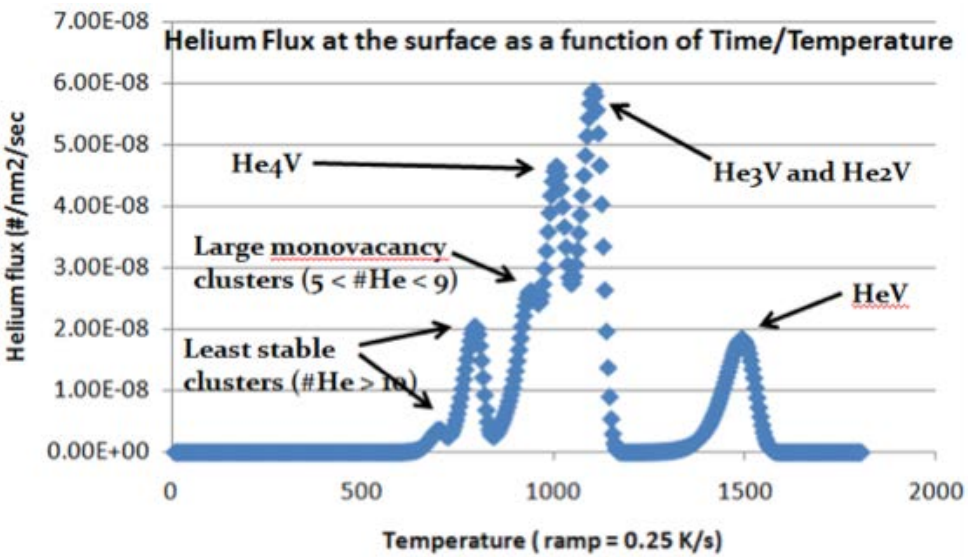
Low energy He implantation of W

Predicted evolution of He clusters below surface during 'irradiation'





Predicted release of He from surface during thermal annealing

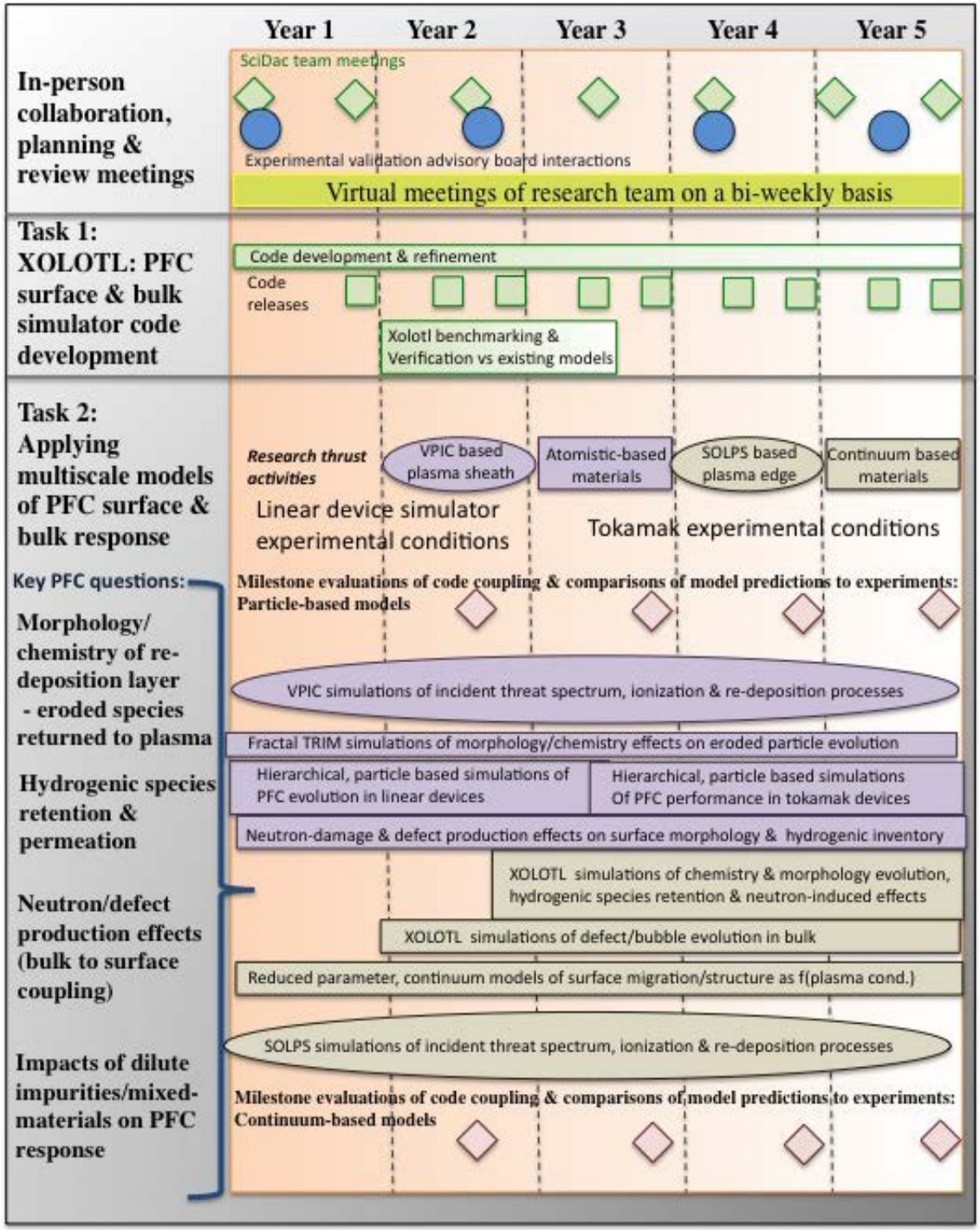


Summary of experimentally observed release peaks following 250 eV He into W

Peak	n_{He}	T_{THDS} (K)	Assigned reaction
H	1	1520	$VHe \rightarrow V + He$
G	2	1220	$VHe_2 \rightarrow VHe + He$
F_2	3	1130	$VHe_3 \rightarrow VHe_2 + He$
F_1	4	1080	$VHe_4 \rightarrow VHe_3 + He$
E	5–9	960	$VHe_n \rightarrow VHe_4 + (n-4)He$

A. van Veen, Materials Sci. Forum 15-18, 3 (1987)

Summary & Future

- PSI SciDAC project provides tremendous opportunity to expand multiscale modeling methodology – from both the 'bottom up' & 'top-down' – to reach physically-relevant time scales of plasma surface interactions thru close integration of SciDAC Institutes and Applied Math/ Computer Scientists with Materials Science and Plasma Physics Domain Scientists

- One focus of project is compiling an experimental validation database & tailoring modeling conditions to match available & new experiments