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

Institution (Lead)	Principal Investigator (Lead)	Additional Personnel
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PNNL	Rick Kurtz	Giridhar Nandipati, Kenny Roche
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UIUC	David Ruzic	Davide Curreli, Kyle Lindquist
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Project web site: https://collab.mcs.anl.gov/display/PSIscidac/

Sponsored by: Fusion Energy Sciences (FES) and Advanced Scientific Computing Research (ASCR)

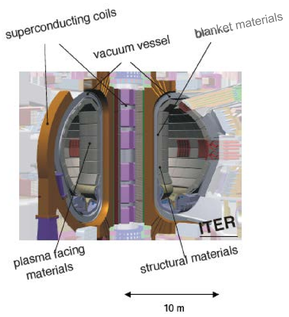
Materials Science Challenges

Materials issues in Magnetic Fusion Energy (ITER/DEMO)

Magnetic fusion energy presents many materials challenges, including:

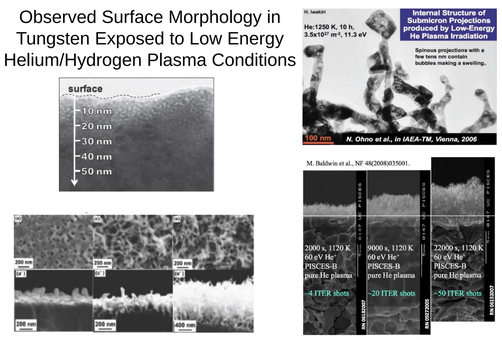
- High thermal heat fluxes
- Erosion/sputtering/blistering of plasma facing components
- Radiation damage
- Low induced radioactivity
- Chemical compatibility
- Joining/welding

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

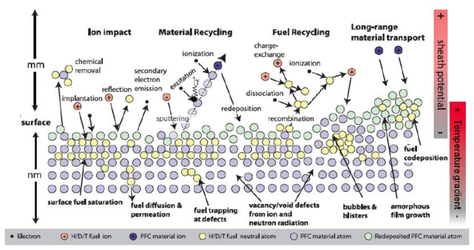


*Ref: H. Bolt, Max-Planck Institute for Plasma Physics, Garching, Germany

Observed Surface Morphology in Tungsten Exposed to Low Energy Helium/Hydrogen Plasma Conditions



Complex, Interlinked Plasma-Surface Interaction Phenomena



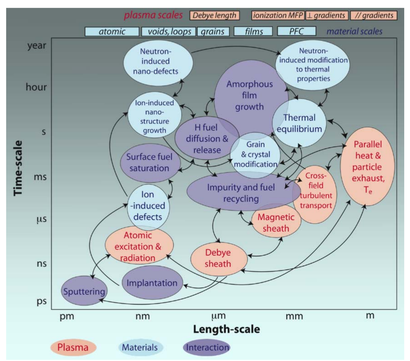


Figure of merit:
Incident plasma ion flux near divertor strikepoint: 10^{24} $m^{-2}s^{-1}$

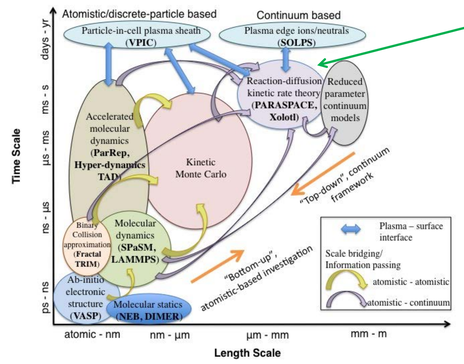
Steady-state sputtering yield O (10^{-4}) on surface monolayer (10^{19} atoms/m^2) results in sputtering of every atom every 0.1 sec -> every atom sputter >10^8 times/year

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

Critical Questions

- What physical parameters control the time dependent evolution of the near-surface morphology and composition in the re-deposition layer (e.g., is this spatial re-deposition zone ever in a steady, or quasiequilibrium, state?)—key phenomena required within predictive modeling include recycling, surface morphology, gas bubble, precipitate and second phase domains, 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;
- The impact of dilute impurities on surface morphology evolution and plasma contamination (e.g., Be in plasma, mixed material transport in tokamaks on erosion/impurity generation); and
- How does the evolving bulk microstructure impact the thermal properties, and thereby feedback into PFC evolution by modifying t he resulting temperature profiles.

Computer Science and Applied Math Challenges



Xolotl-PSI – A 3D Continuum Reaction-Diffusion Kinetic Rate Theory Plasma-Surface Interaction Code

- Xolotl is the Aztec god of lightning and death, pronounced SHO-lottle
- To be developed from scratch by this project
  – Extending ideas in 1D prototype (PARASPACE)
- Design for HPC – current and emerging architectures
  – Multicore, multicore+accelerator
- Integrate performance measurement, in situ analysis and visualization at design time
  – Design in resilience features: checkpoint/research and more
- Expect to leverage PETSc, MOAB, Visit, TAU, mpiP, …
  – Also look at products of X-Stack Research projects
- Proposed programming environment:
  – C++, MPI, OpenMP, OpenACC (expect some CUDA/OpenCL also)

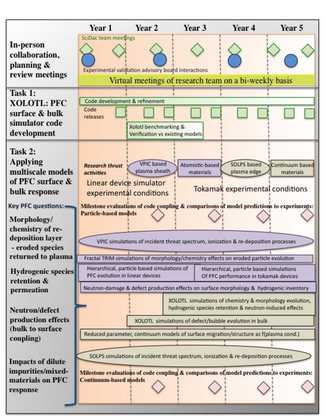
Existing Lower Length-Scale Codes

- Plasma interface: SOLPS, VPIC, LAPS
- Micro-structural evolution: OR-RIME
- Kinetic Monte Carlo: PNNL KMC, SEAKMC
- Accelerated molecular dynamics: TAD, AMDF
- Molecular dynamics: LAMMPS
- Density functional theory: VASP
- Performance and scalability
- Uncertainty quantification
- Analysis and visualization for understanding

Critical Questions

- Scalable algebraic and geometric multigrid methods for 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 Institute (SDAV).

Proposed Project Milestones and Timeline



	Year 1	Years 2-3	Years 4-5
Task 1 - Development and Refinement of the Xolotl PFC Simulator	• Initial Xolotl development for 3D evolution of tungsten-surfaces exposed to D, He and Be plasmas, to be 'loosely coupled' to SOLPS • First code release at end of year 1.	• Refine Xolotl through evaluation of IMEX solvers and scaling studies; • Evaluate more extensive coupling across the plasma - materials interface; • Benchmark and verify Xolotl.	• Refine and extend Xolotl for expanded number of unknowns to account for additional species and larger spatial scales for tokamak condition modeling.
Task 2 - Applying and Integrating Multiscale Materials Models to Predict PFC and Bulk Materials Response to Burning Plasmas	• VPIC evaluation of plasma exposure conditions in PISCES for determining input parameters to atomistic modeling; • Initiate MD/Fractal-TRIM/AMD simulations of tungsten surface exposure in the low-temperature regime; Initiate atomistic studies to evaluate sub-surface radiation damage evolution; • Initiate reduced parameter continuum models to evaluate surface porosity and gas bubble effects on erosion/sputtering rates and surface growth; and Devise UQ implementation strategy.	• Initiate KMC simulations of low-temperature tungsten surface response and feedback evolving surface structures to VPIC; • Continue MD/Fractal-TRIM/AMD simulations for evolving tungsten surface at low-temperature and initiate simulations in the higher-temperature regime; • Initiate studies of sub-surface defect evolution and coupling with KMC to evaluate impacts on D retention; • Initiate Xolotl modeling of tungsten surface exposure in the low-temperature regime; • Continue continuum level models to evaluate surface morphology in low versus high-temperature regime; • Comparison of multiscale modeling to experimental observations; and • Implement UQ analysis and error propagation across scales.	• Initiate atomic-scale simulations and plasma - materials interfacing for tokamak exposure conditions; • Coupled KMC - VPIC simulations of high-temperature tungsten surface response and feedback in PISCES experiments with pre-radiation damaged materials; • Implement UQ analysis of importance of coupled reaction terms in Xolotl for predicted response; • Initiate Xolotl modeling in the high-temperature PISCES regime, with coupling to SOLPS, and for tokamak exposure conditions, with coupling to VPIC; • Comparison of multiscale modeling to experimental observations for tokamak conditions; and • Evaluation of advantages and disadvantages of atomsitic (KMC) versus continuum (Xolotl) methods for long-term PFC evolution.