Case study: Plasma – Materials Interactions

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Presentation Overview

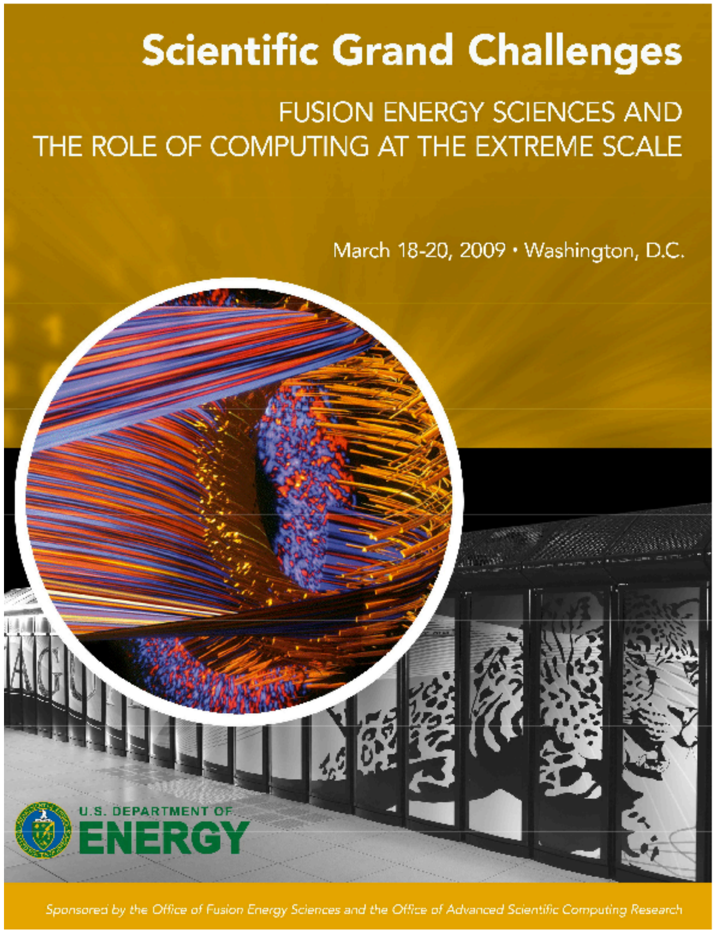
- Challenges of plasma facing components & structural materials in the (magnetic) fusion environment

- Multiscale phenomena governing materials changes & performance, and the multiscale modeling approach
  - Still very much a work in progress – no single, integrated code
  - Much of the modeling is performed on smaller, individual PI clusters

- Select set of codes, results and computing requirements

- Summary and future work

Fusion Materials Challenges



Co-chaired by Bill Tang and David Keyes

Plasma Materials Interaction Science Challenges:

Modeling the edge and scrape-off layer plasmas. *This includes modeling of turbulent transport and full coupling of plasma ions and electrons, neutrals, photons, and electromagnetic fields. In addition, plasma contamination from near-surface transport of sputtered or vaporized material and quantification of plasma facing component particle and photon fluxes (with predictions of instability regimes) should be considered.*

Predicting the near-surface material response to the extreme plasma fluxes of photons and particles under normal and transient operation*. This includes predicting sputtering erosion/re-deposition and other time-integrated plasma facing component processes (e.g., dust formation and transport; helium- or deuterium-tritium-induced microstructure formation and flaking) and the resultant impurity transport, core plasma contamination, mixed-material formation, and tritium co-deposition in redeposited materials. The material and edge plasma response to transient processes such as high-powered edge localized modes vertical displacement events, plasma disruptions, and runaway electrons represent an important component of this effort.*

Modeling the underlying structural materials response. *This involves understanding the fundamental microstructure evolution and performance limits of structural materials in the fusion radiation environment that involve extreme cyclic thermo-mechanical stresses and simultaneous intense fusion neutron bombardment.*

An overarching grand challenge will involve efficient integration of these to develop a comprehensive model.

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

- **Magnetic fusion energy presents many materials challenges, including:**
  - High thermal heat fluxes

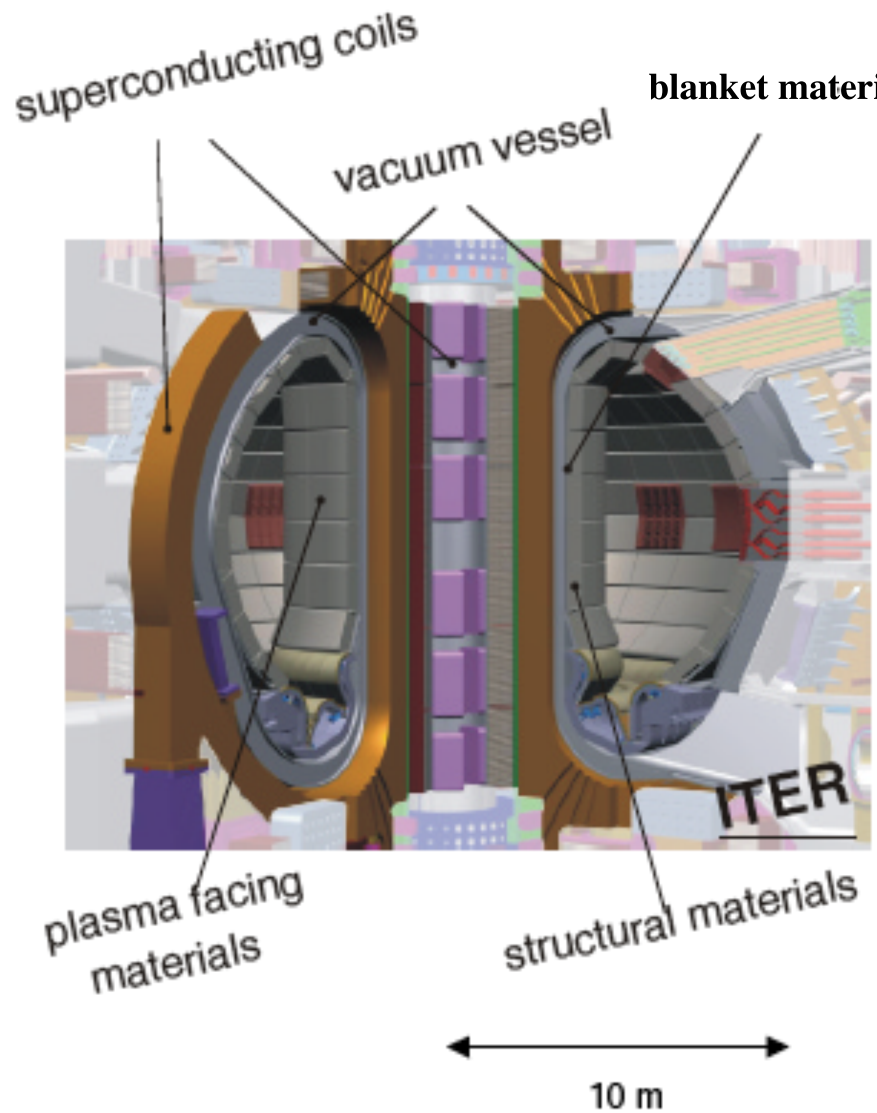
  - Sputtering/blistering of plasma facing components

  - Radiation damage

  - Low induced radioactivity

  - Chemical compatibility

  - Joining/Welding



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

*Plasma Facing Components/Materials (ITER)**

<u>Key issues</u>

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

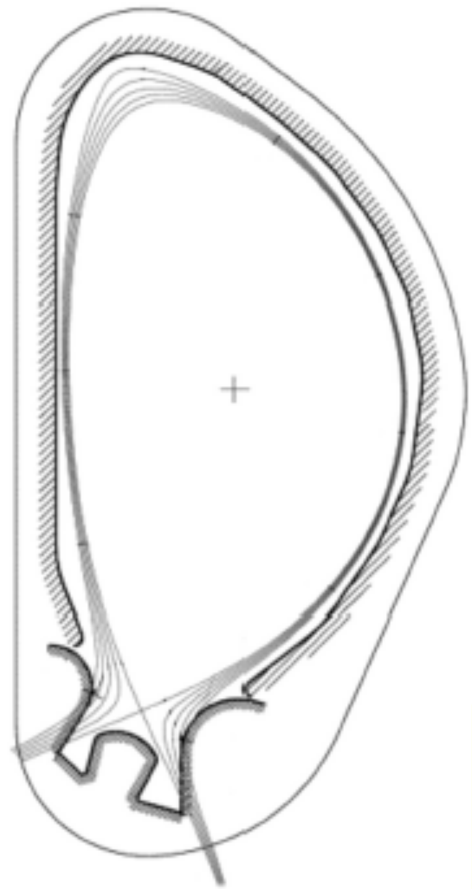
<u>Leading candidate materials</u>

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

<u>transient heat loads</u>:

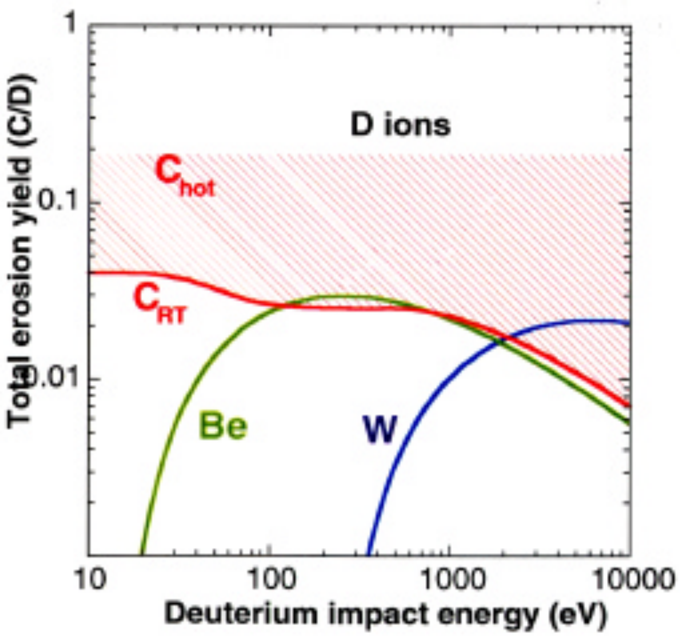
e.g. ELMs, disruptions

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

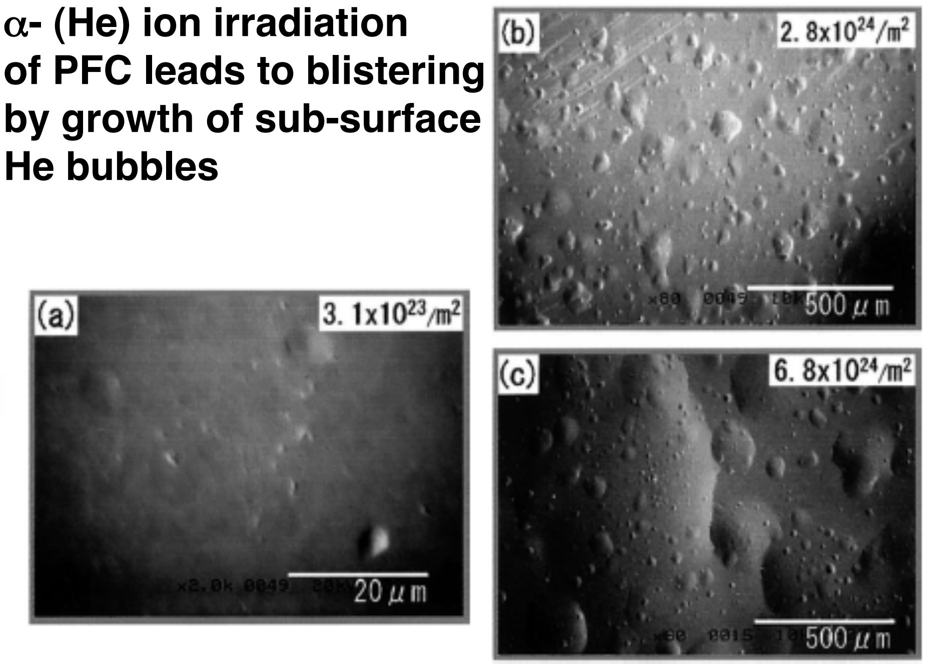
*PFC Materials: Erosion & Blistering of C, Be & W**

- Neutron irradiation of C leads to decreases in thermal conductivity

First wall:
Erosion of
low Z materials
order of 3 mm/burn year: 15 mm in 5 years
tungsten
order of 0.1 mm/burn year: 0.5 mm in 5 years



Blistering:**
α- (He) ion irradiation of PFC leads to blistering by growth of sub-surface He bubbles

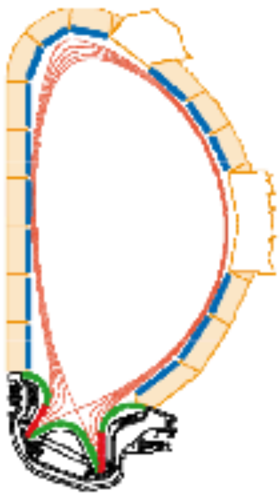


Divertor:
mostly redeposition of eroded wall material

Presently: order of magnitude-knowledge;
data from ITER needed to assess PFM thickness

Ref: * H. Bolt, Max-Planck Institute for Plasma Physics, Garching, Germany
** T. Shimada, Y. Ueda, M. Nishikawa, *Fusion Eng. & Des.* ***66-68*** *(2003) 247*.

*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. carbides, oxides, 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).

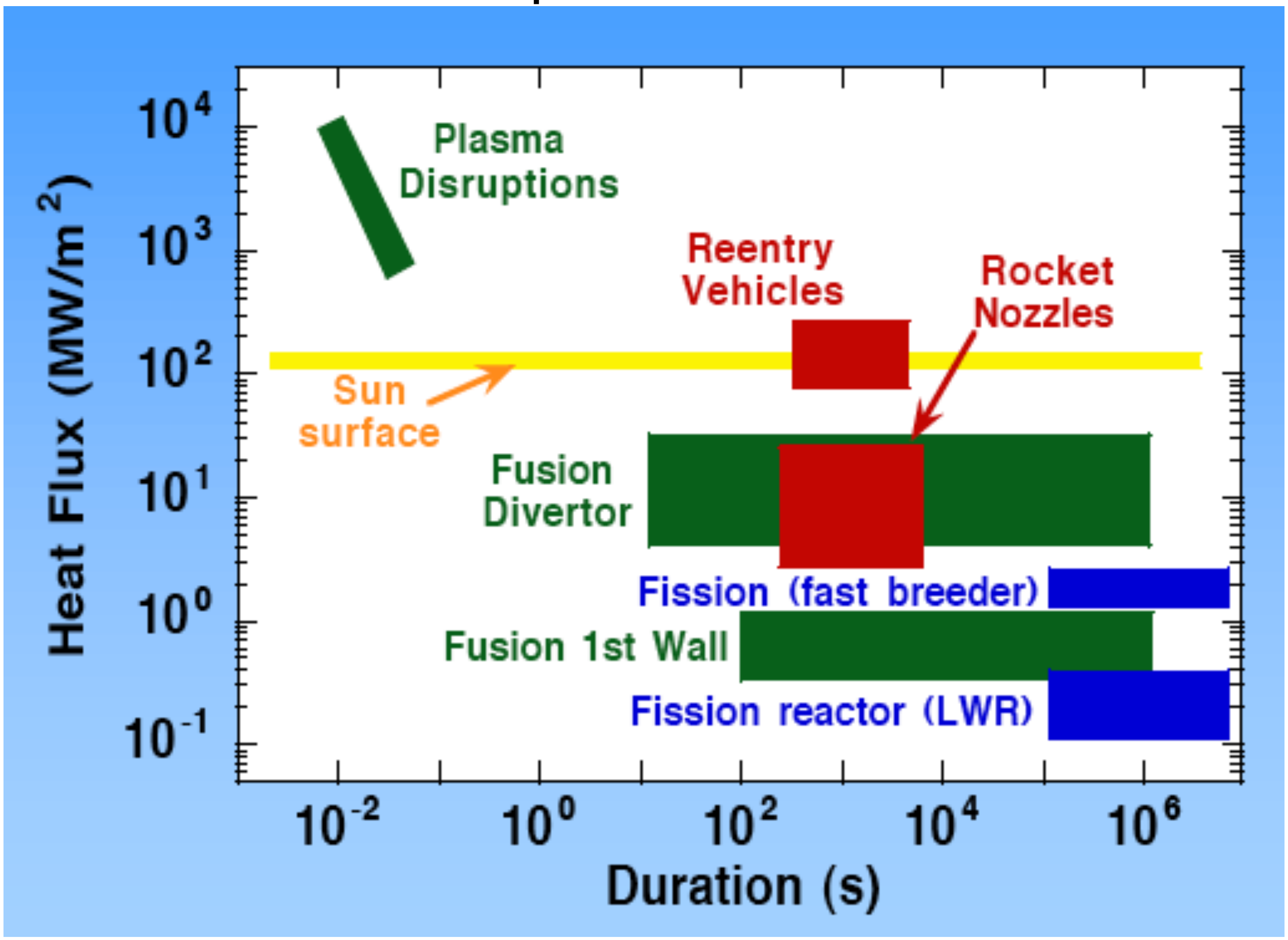
*PSI extrapolation challenges **

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

* D. Whyte, IHHFC, Dec 2008

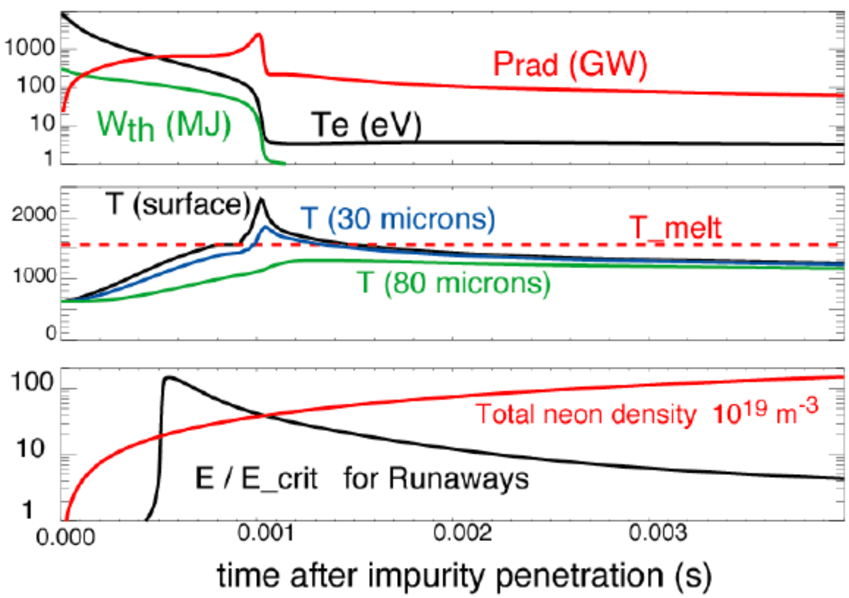
*Fusion materials challenges: Heat flux**

Comparison of Heat fluxes

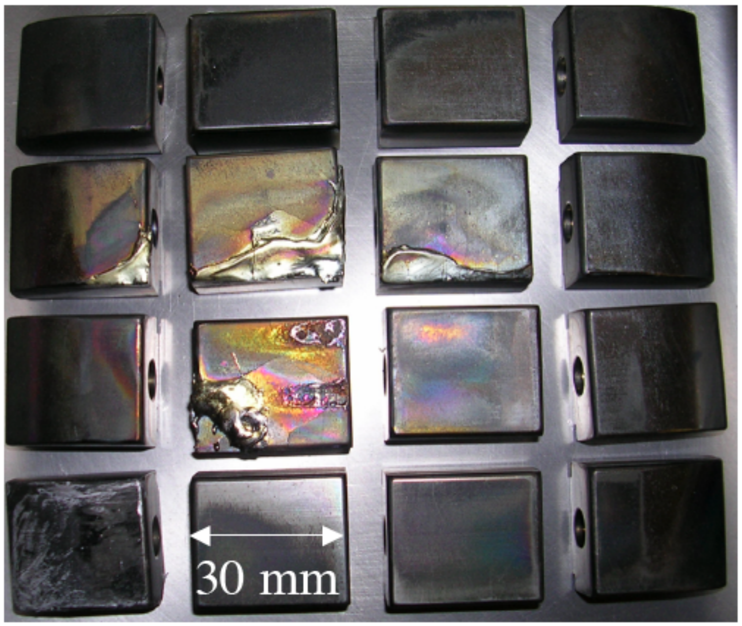


* **S.J. Zinkle**

*High thermal heat fluxes – transients evolve over ms**



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 == $N_{e,ITER}$

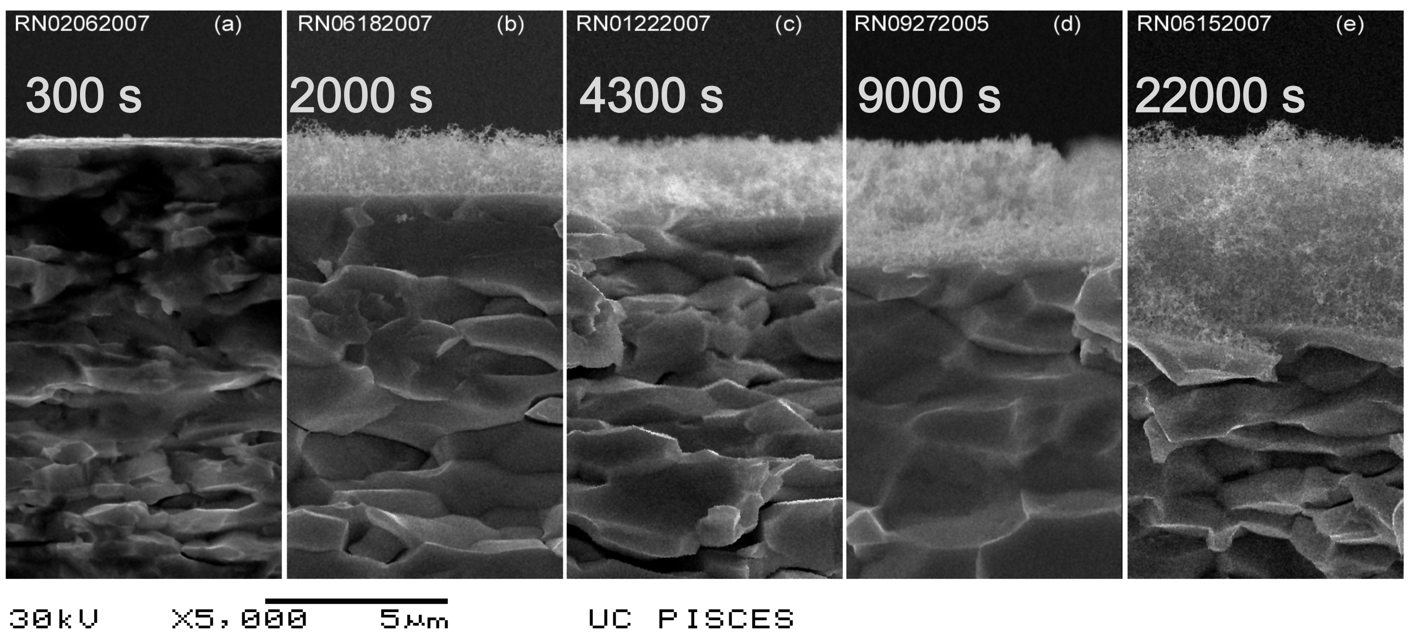
* D. Whyte, IHHFC, Dec 2008

*Combined thermal and particle fluxes**

Dust formation in ITER PFC mix from several possible sources*:

- Deposited layer disintegration under transient loads → most likely in divertor were layers most likely to grow
- He-induced nano-morphology → dust formation in steady state, enhanced "non-atomistic" erosion rates on W

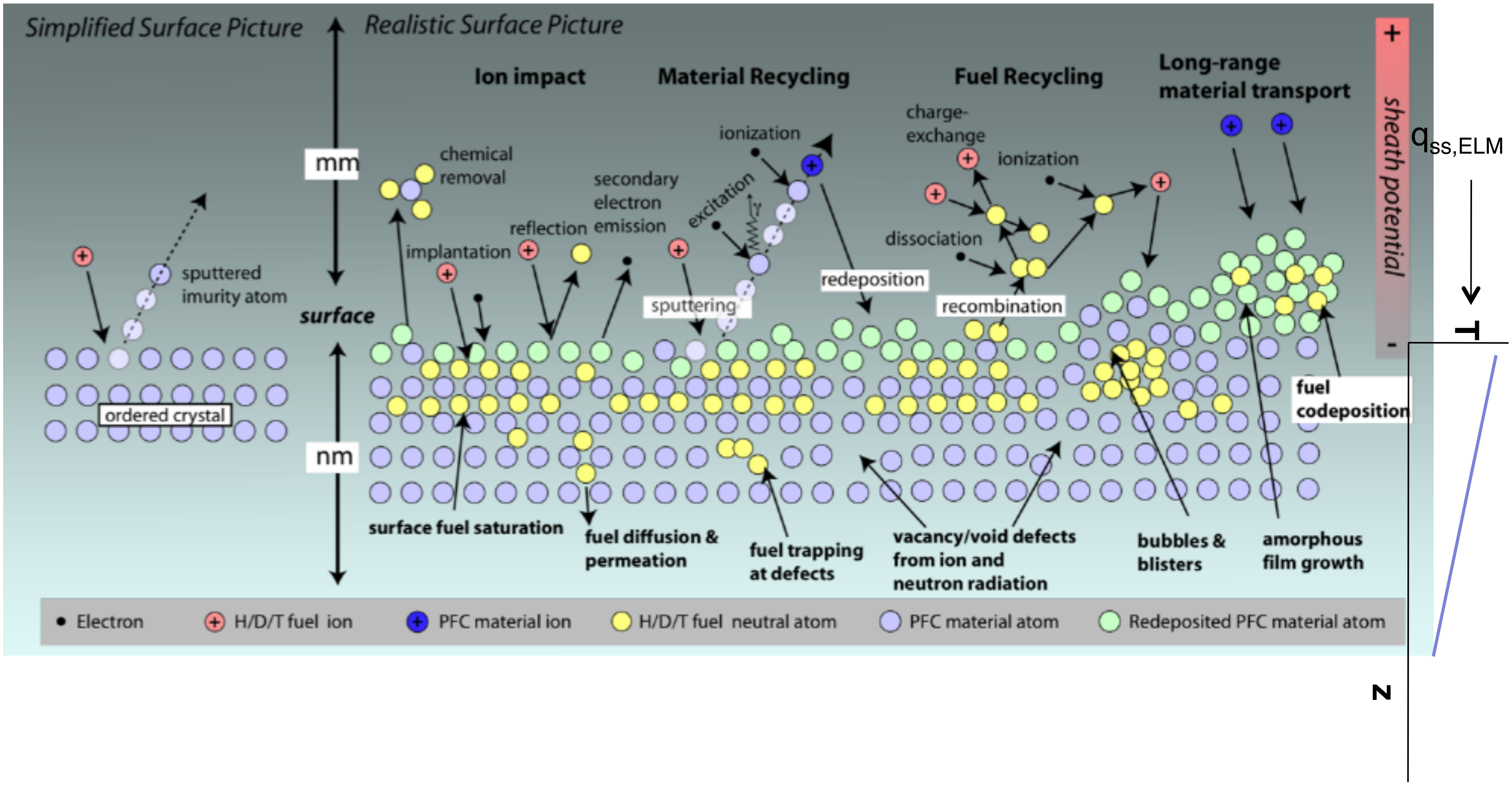
M. J. Baldwin et al., PSI 2008



T_s = 1120 K, Γ_{He+} = 4–6×10^{22} m^{-2}s^{-1}, E_{ion} ~ 60 eV

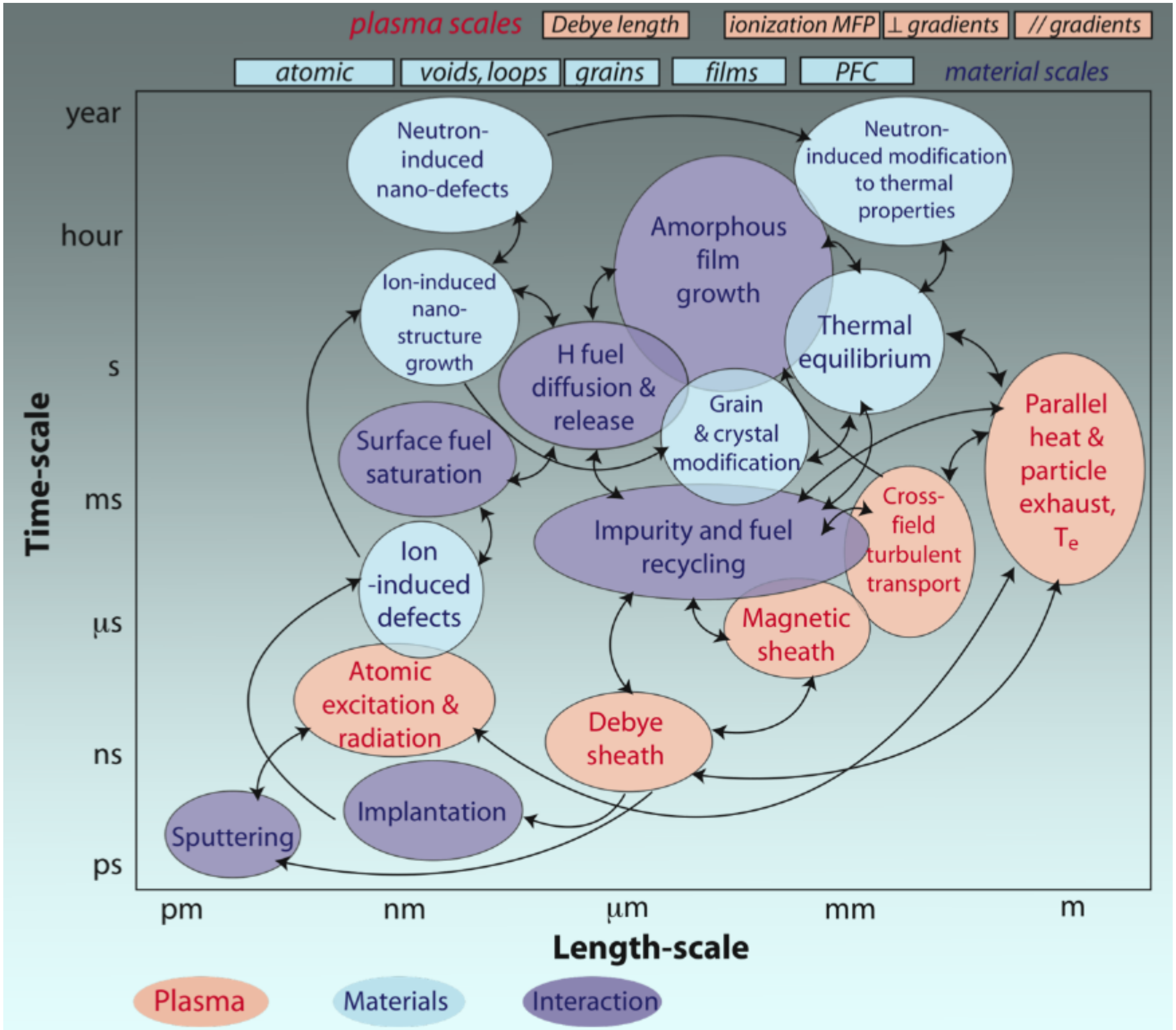
* R.A. Pitts, IHHFC Workshop, Dec 2008

*Complex, interlinked PSI phenomena**



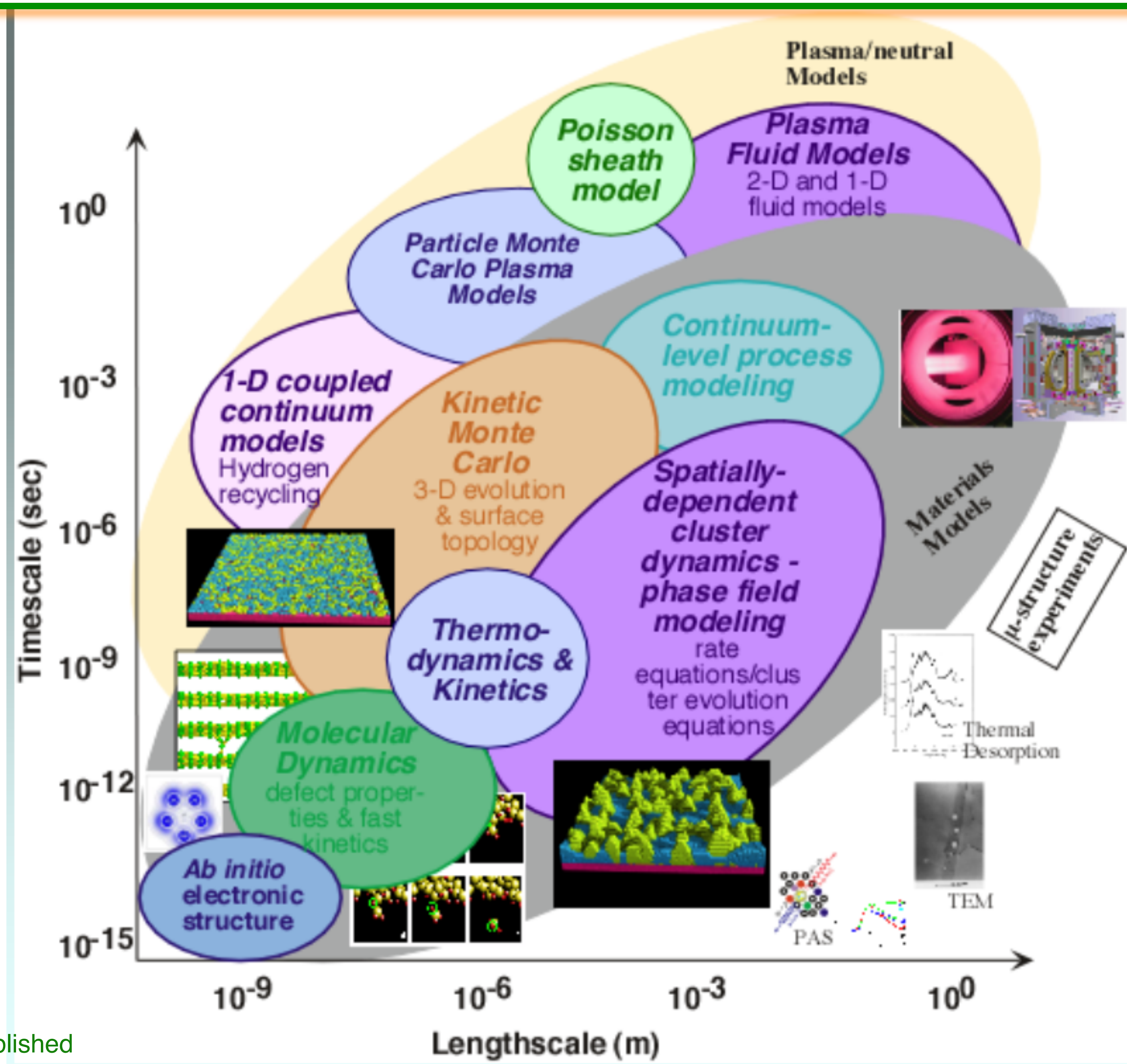
* Whyte and Wirth, unpublished

*Multiscale, interlinked Plasma-Surface Interaction phenomena**



* Whyte and Wirth, unpublished

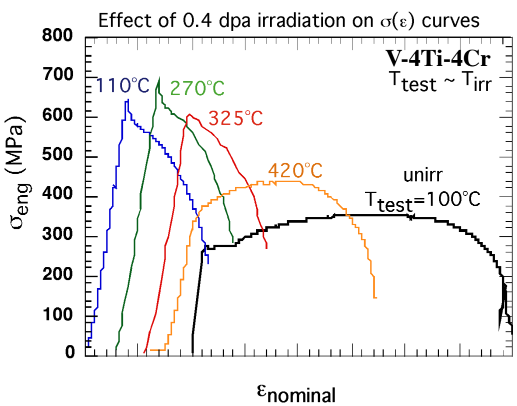
*Multiscale modeling capability – a work in progress**

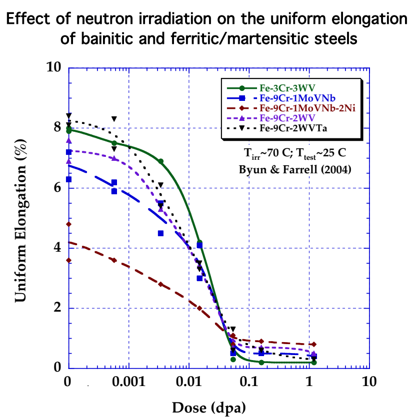


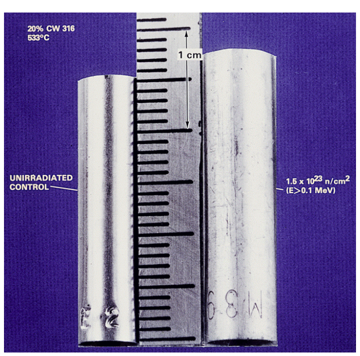
* Whyte & Wirth, unpublished

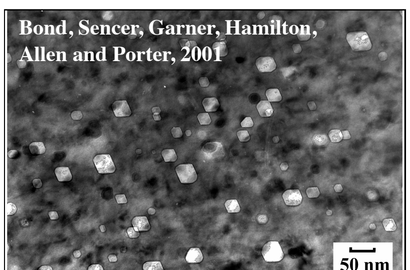
Irradiation effects on structural materials

- Exposure to neutrons degrades the mechanical performance of structural materials and impacts the economics and safety of current & future fission power plants:
  - Irradiation hardening and embrittlement/decreased uniform elongation (< 0.4 T_m)
  - Irradiation (<0.45 T_m) and thermal (>~0.45 T_m) creep
  - Volumetric swelling, dimensional instability & growth (0.3 - 0.6 T_m)
  - High temperature He embrittlement (> 0.5 T_m); Specific to fusion & spallation accelerators
- Additional environmental degradation due to corrosive environments (SCC, uniform/shadow corrosion, CRUD)









304 Stainless steel irradiated in EBR-II, 380°C, ~22 dpa, 1% swelling

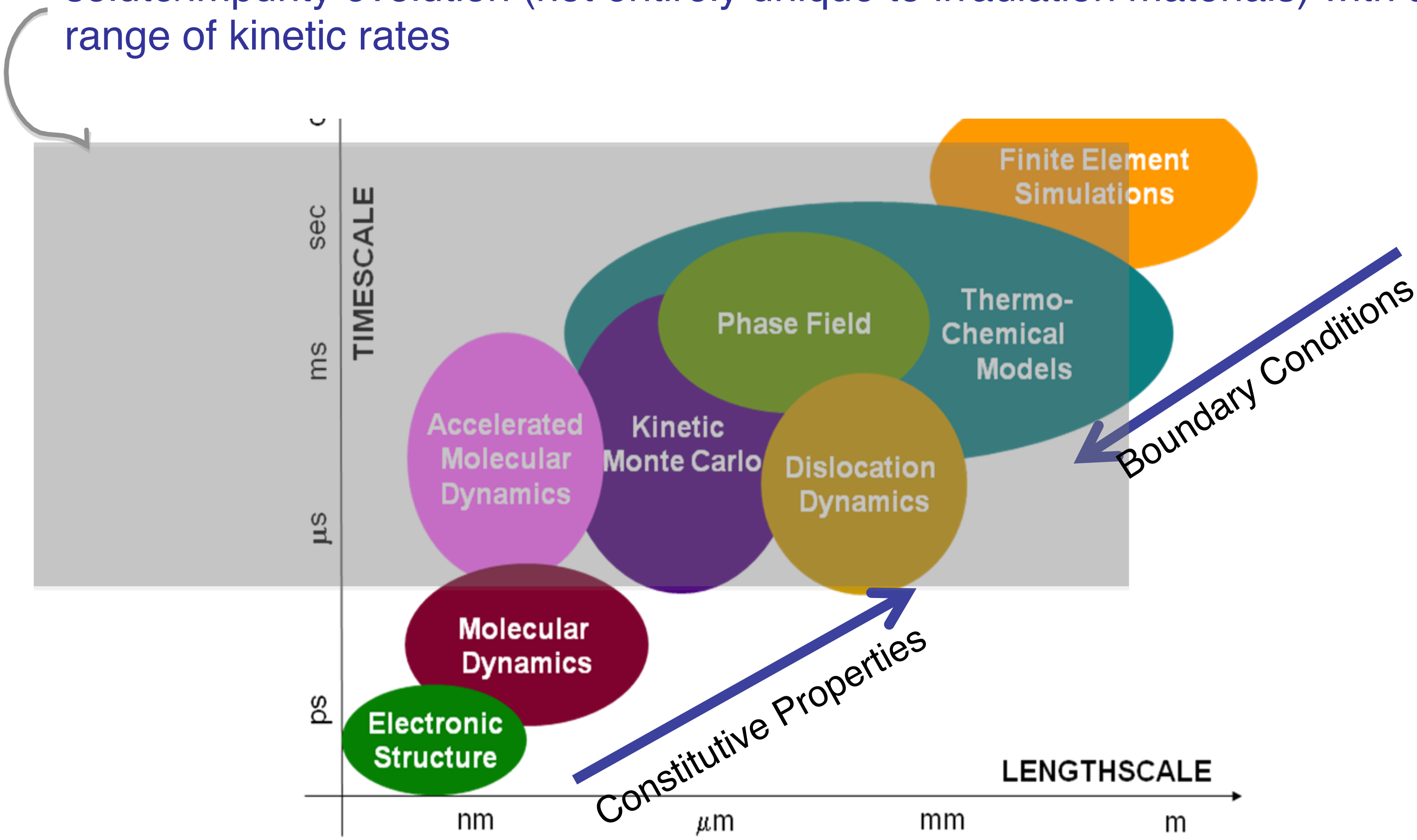
Variables

- Structural Materials (Fe-based steels, Vanadium and Ni-based alloys, Refractory metals & alloys, SiC) and composition
- Zr alloy cladding
- Initial microstructure (cold-worked, annealed)
- Irradiation temperature
- Chemical environment & thermal-mechanical loading
- Neutron flux, fluence and energy spectrum
  - materials test reactor irradiations typically at accelerations of 10^2 - 10^4

Synergistic Interactions

Multiscale modeling approach – structural materials

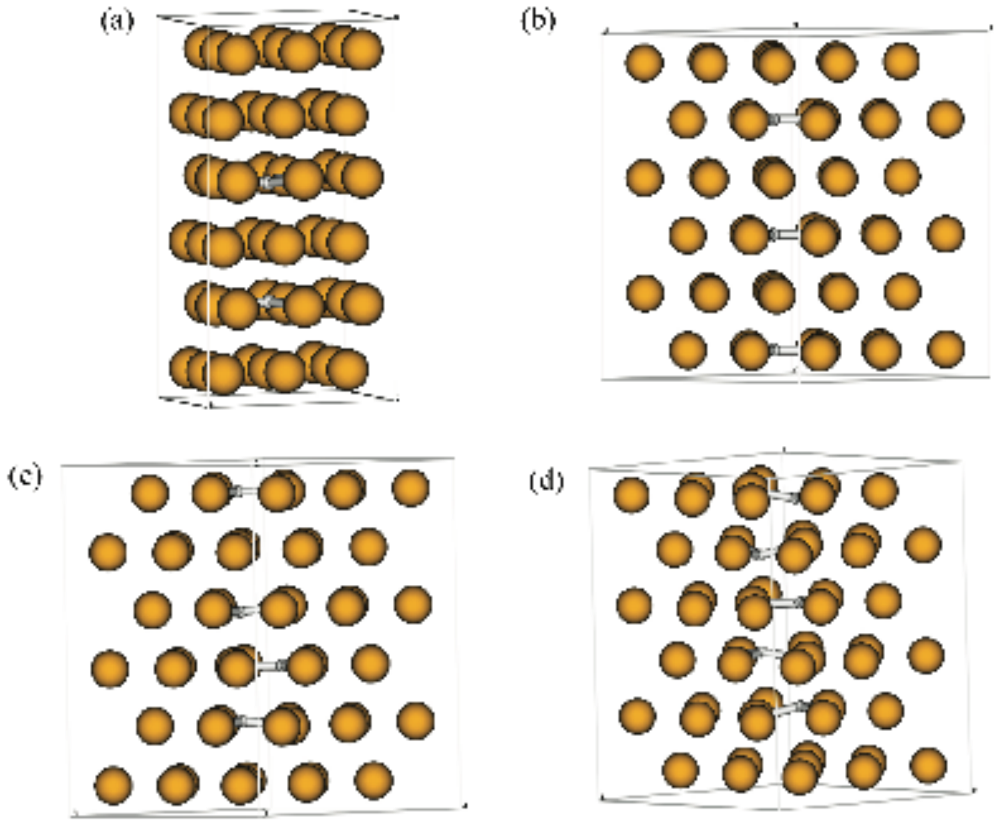
Our biggest scientific challenge is understanding the kinetics of coupled defect – solute/impurity evolution (not entirely unique to irradiation materials) with a wide range of kinetic rates



Electronic structure calculations

- **'Common' electronic structure codes: Abinit, Quantum Espresso, VASP**

  Example – H clusters in Beryllium*



Density Functional Theory applications to investigate structure and energetics of Plasma surface interactions

Generally scale well up to 1000's of processors

* A. Allouche, M. Oberkofler, M. Reinelt, and C. Linsmeier, *J. Phys. Chem.* C 114 (2010) 3588-3598.

Molecular Dynamics calculations

- **'Common' MD codes: LAMMPS, SPASM**

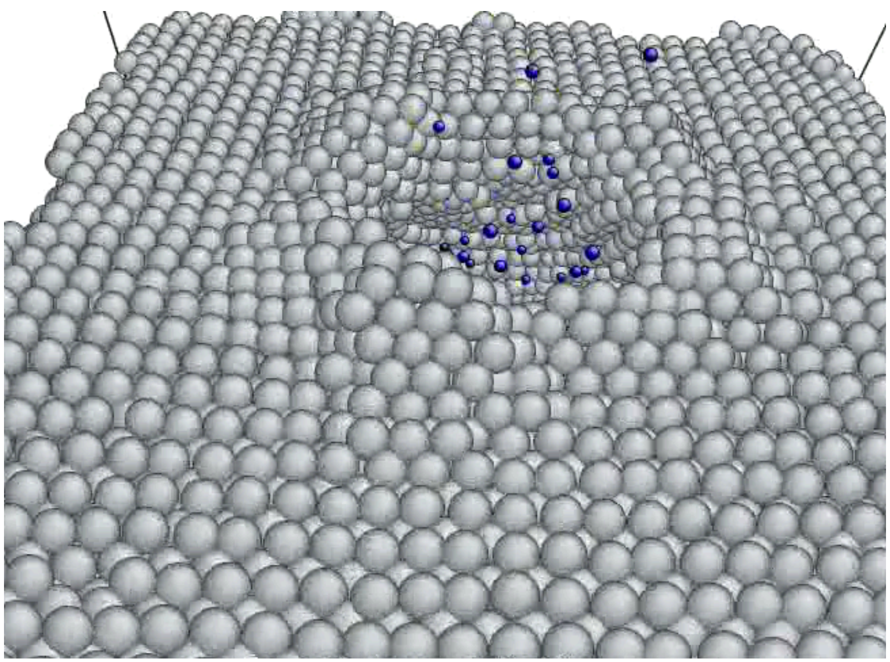
  - typically run on small, clusters (usually because of throughput), especially for 'discovery' science

  - LANL has demonstrated SPASM for 1 billion atoms for 1 nanosecond

- **Accelerated MD codes**

  - LANL demonstrated Parallel Replica Dynamics on 1000 atoms and 12,000 replicas

Bursting of He bubble onto W surface

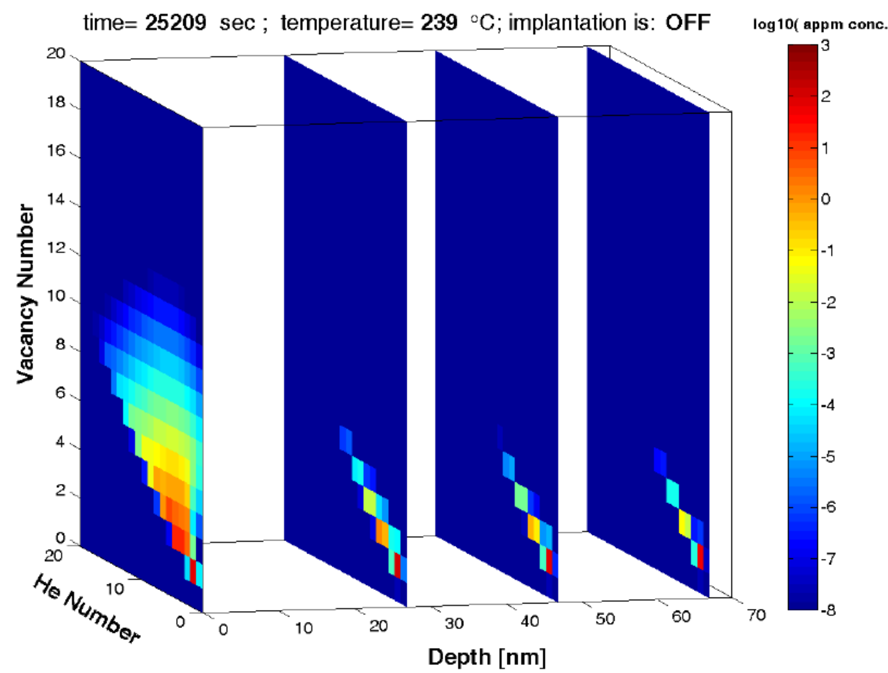


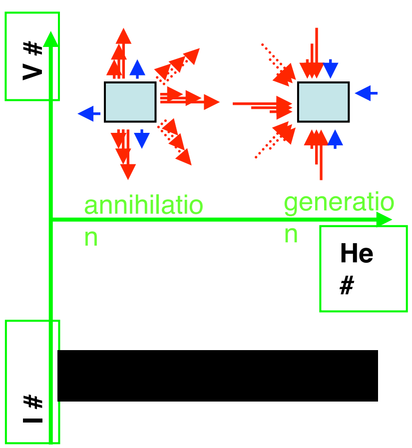
Road Runner experience (SPASM):

Flop count: petaflop
core-hour per run: 2.8 million
number of cores: 120,000
wall clock time: 24 hours
total memory: 12000 GB
minimum memory per core: 0.1 GB
total data read & written per run: 100 GB
size of checkpoint file: 0.1 GB

Spatially-dependent cluster dynamics model

- *Dimensionality*
  1 spatial dim.: x, non-uniform grids
  1 temporal dim.: t, non-uniform grids
  1.5 phase-space dims: He#, V(I)#
- *What kind of transitions?*
  Any cluster can annihilate (transform to another) or be created (transformed from another) :
  - Capturing: all directions, all step sizes possible, depending on existing mobile species; ***including bubble coalescence***
  - Dissociating: single He, V, I, only





Calculations can involve > 10^7 coupled reaction – diffusion differential equations – utilize parallel solvers (PARDISO)

$$\frac{\partial[He_i]}{\partial t} = D\frac{\partial^2[He_i]}{\partial x^2} + \text{dissoc.\_rate}(He_m V_n) + \text{He\_kickout\_rate}(HeV) + \text{implan.\_rate} - \text{self\_trap\_rate} - He_i\text{\_trap\_rate}(He_m V_n) - \text{annihilation by dissociation}$$

PARASPACE Model construction

- **How to describe the rates?**
  - capture: C1+C2 → C3;

$$R_{+,1,2} = k_{+,1,2}[C1][C2]; \quad k_{+,1,2} = 4\pi(r_1 + r_2)(D_1 + D_2) \text{ (×Bias, if both interstitial type)}$$

$$r_{(V_n)} = n^{1/3} r_a \qquad r_{(I_n)} = \sqrt{\frac{nV_a}{\pi b}} \qquad D = D_0 \exp(-E_m / k_B T)$$

  - dissociation: C3 → C1+C2;

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

- **Boundary conditions (BC)**
  black BC, i.e., all concentrations are zero on the surfaces

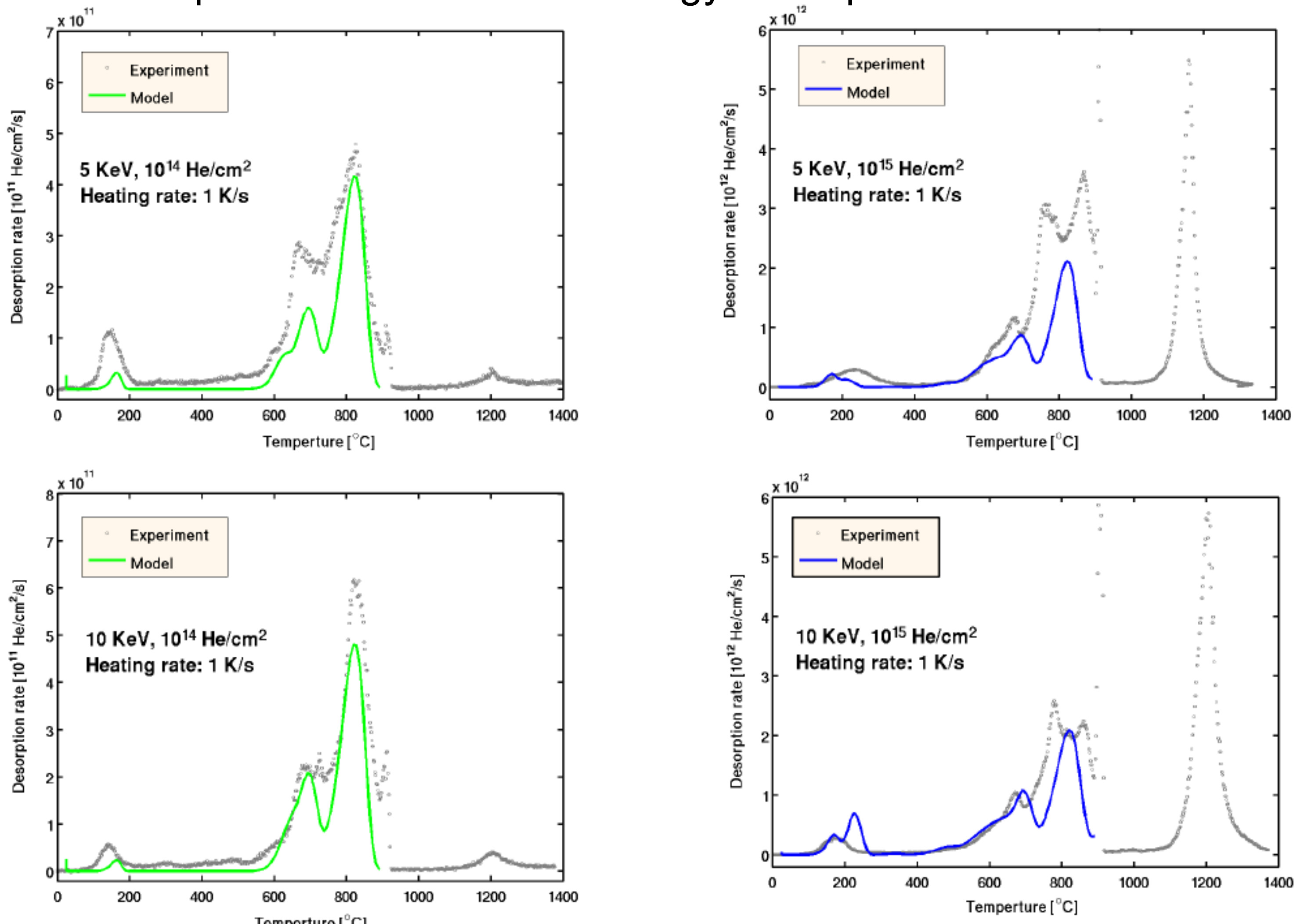
- **Spatial derivative (finite difference)**

$$\frac{\partial^2 C_i^{x_n}}{\partial x^2} = \frac{\frac{(C_i^{x_{n+1}} - C_i^{x_n})}{x_{n+1} - x_n} - \frac{(C_i^{x_n} - C_i^{x_{n-1}})}{x_n - x_{n-1}}}{(x_{n+1} - x_{n-1})/2}$$

- **Parallel, large sparse-matrix linear solver (PARDISO) using open-MP formalism and backward difference time integration - easily treat systems with 10^7 degrees of freedom**

Spatially-dependent rate-theory based modeling

- Thermal desorption behavior of low-energy He implanted into iron

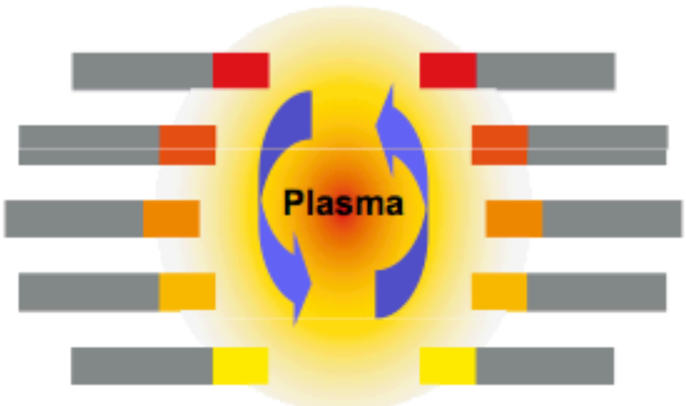


- **Model reproduces (major) desorption groups & approximate peak Temp's**
- **Model overestimates He-leakage during room T relaxation**

Xu and Wirth, *J. Nucl. Mater.*. **403** (2010) 184.

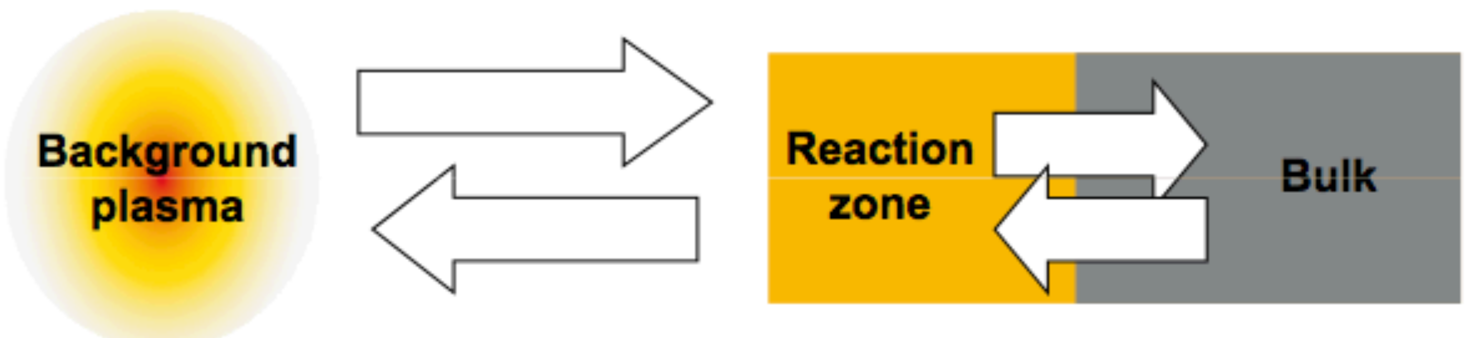
*Spatially-dependent reaction-diffusion modeling**

Treat complex **plasma-wall interactions** and **material evolution** in a simplified way



Analytical model:

- first wall: *n* tiles, different loads
- background plasma (B2 + EIRENE …)
- redistribution matrix (DIVIMP)
- SDTrim sputter yields
- parametrized surface materials evolution



* C. Linsmeier, PSI-19 invited presentation

Summary & Future Challenges

• Fusion materials performance is an inherently multiscale challenge – significant effort ongoing to utilize multiscale materials modeling and high performance computing – but this is in the early stages of research and implementation – lots of effort at different scales, few (none) integrated codes using high-performance computing

• Key techniques for 1000's of core processing are density functional theory (Abinit, Quantum Espresso, VASP)
• Molecular dynamics simulations widely used – but predominately at the individual computing cluster level
• Reaction-diffusion solution approaches being developed for defect/surface/chemistry evolution -> will eventually be the large-scale, high performance computing platform to integrate with edge plasma modeling
• Monte Carlo approaches are also being pursued – and particle in cell models for the near surface plasma ionization response (LANL VPIC demonstrated at petaflop scales)

• Continuing development of knowledge and models through Fusion Simulation Project, etc. leading to increased modeling investigation of Plasma Surface Interactions and Bulk Fusion Materials investigation