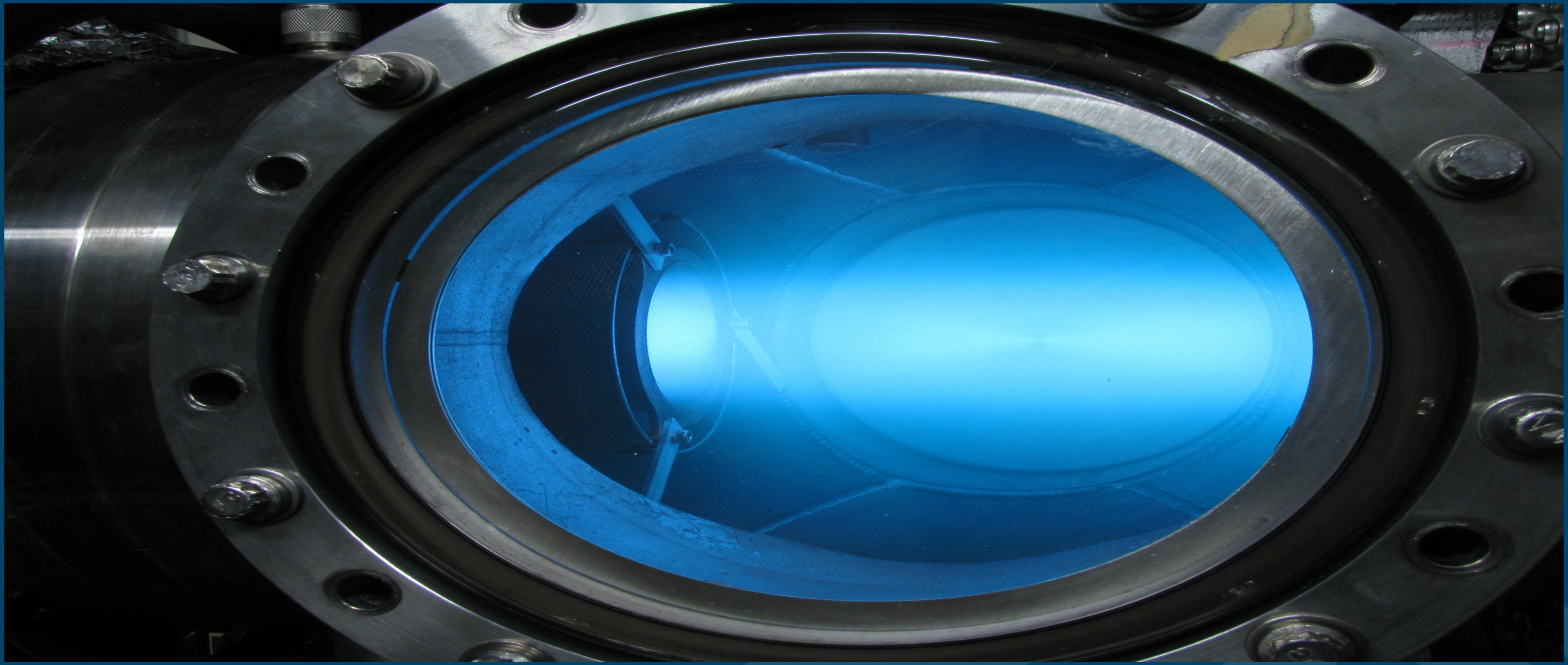
# Plasma-material interactions in magnetic fusion devices

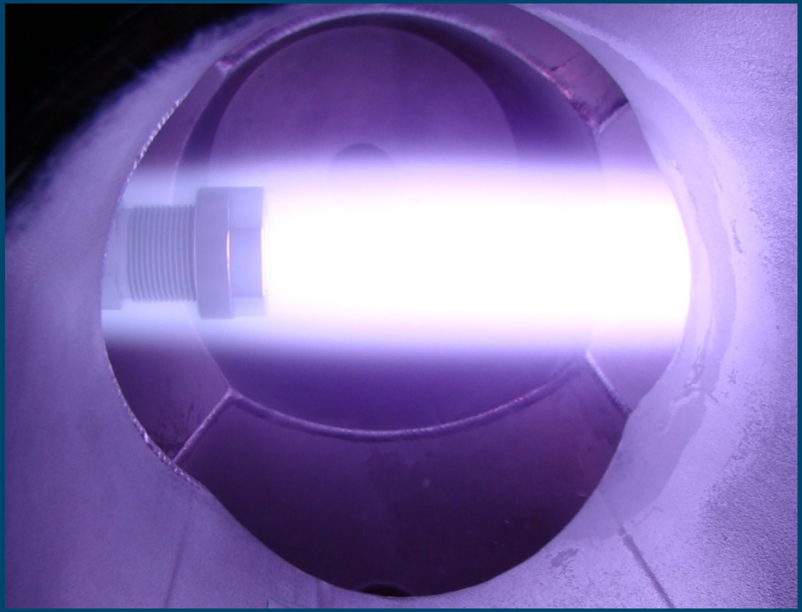


Robert Kolasinski
*Sandia National Laboratories, Livermore, CA*
*Chemistry, Combustion & Materials Center*

SULI Introductory Course in Plasma Physics / PPPL / June 16, 2017

# Outline

- The magnetic fusion program at Sandia
- Underlying physics of plasma-materials interactions (PMI)
  - PMI experimental techniques
  - Simulation tools
  - Recent research directions
- Advanced concepts



# Hydrogen in materials research at Sandia/CA

**Chemistry, Combustion, & Materials Center**

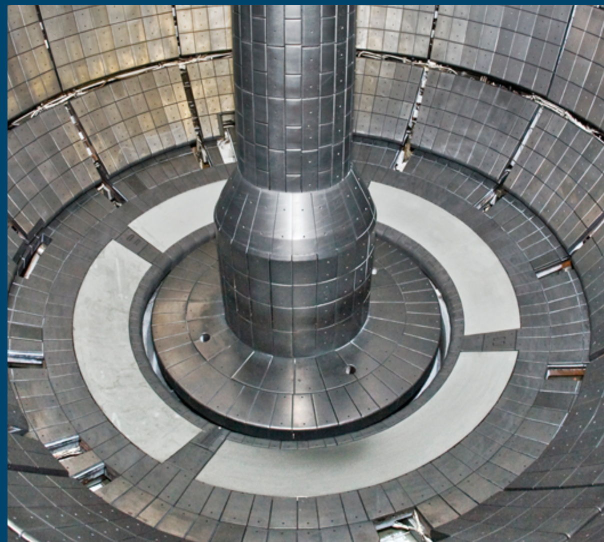
- ~200 research staff

**Combustion Research Facility**

Office of Science-funded DOE user facility

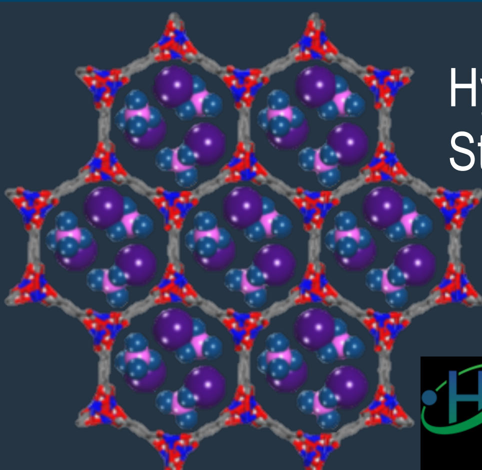
Livermore Valley Open Campus (SNL-LLNL)

# Hydrogen in materials research at Sandia/CA



Magnetic Fusion Energy

Hydrogen Effects on
Structural Materials



Hydrogen
Storage

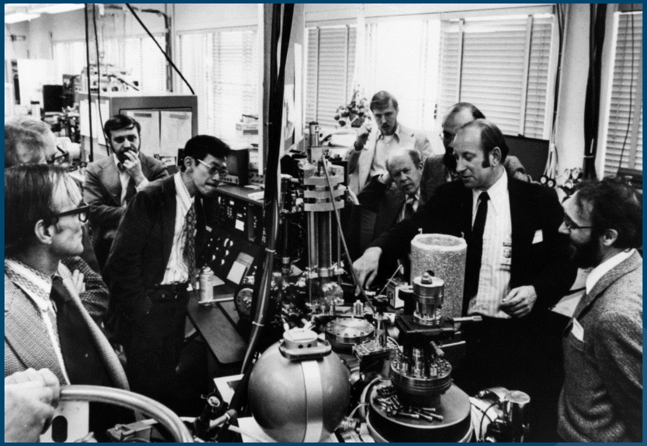
HyMARC

Fuel Cell
Electric Vehicle
Infrastructure

# Magnetic fusion research at Sandia/CA

- Sandia scientists have made fundamental contributions to hydrogen science and PMI

Inventors of the **embedded atom method**: Mike Baskes, Murray Daw, and Stephen Foiles (1982)

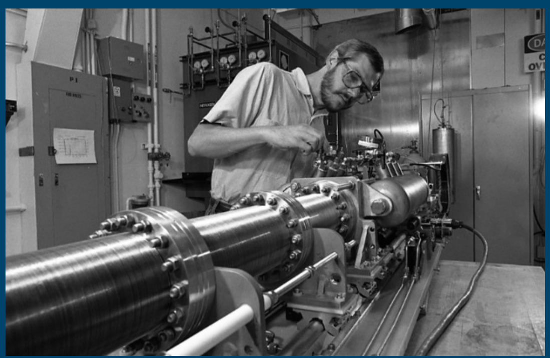


Walter Bauer gives a tour of Sandia/CA's ion beam laboratory during the 2nd PSI meeting (1976)

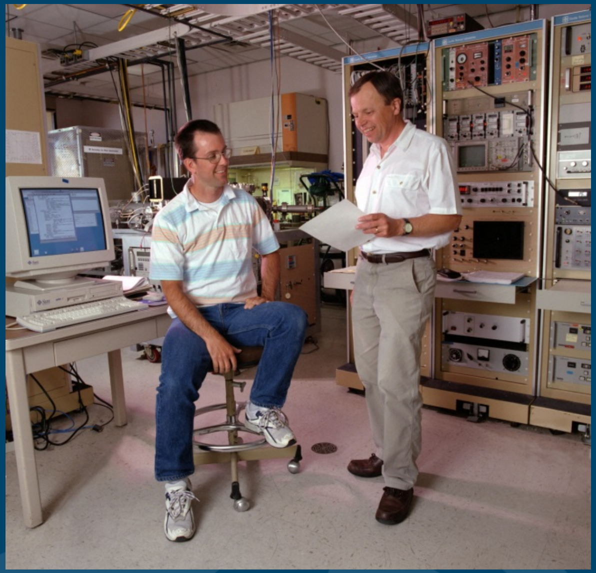
Repulsive **interatomic potentials** developed at Sandia formed basis for TRIM model (1980)

# Magnetic fusion research at Sandia/CA

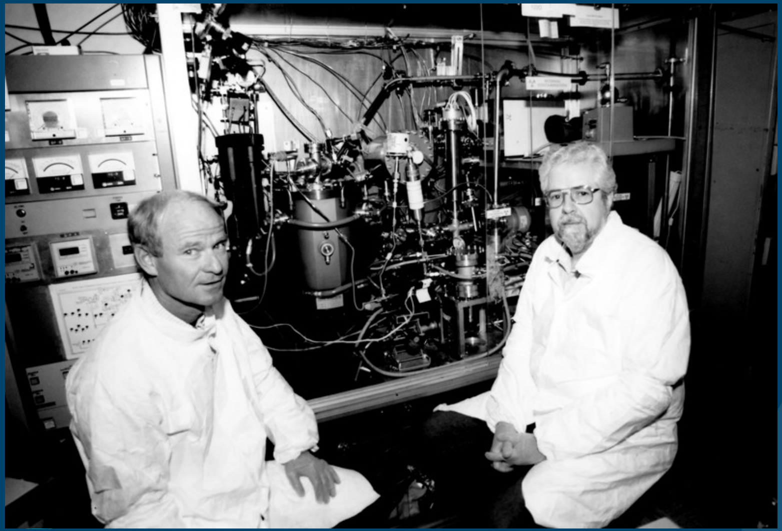
- Sandia scientists have made fundamental contributions to hydrogen science and PMI



**Innovative plasma diagnostics:** Jonathan Watkins inspects a fast-scanning probe for installation on DIII-D (1990)

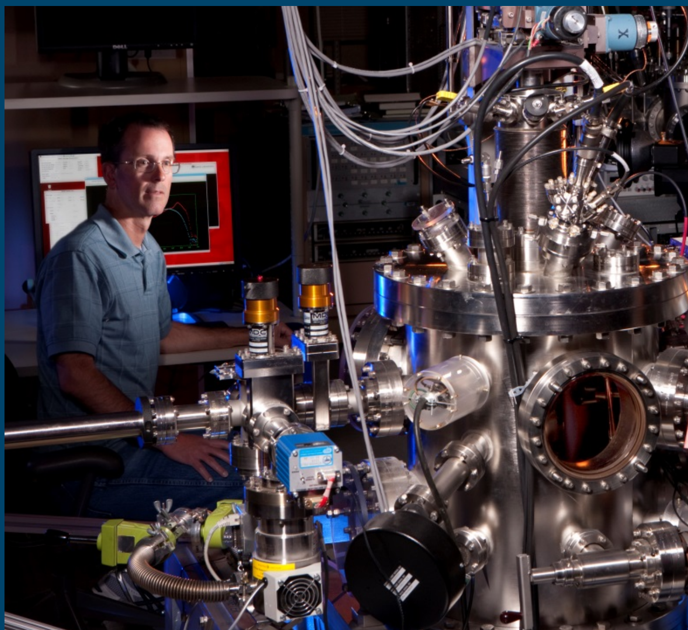


**Characterization of liquid metal surface composition; hydrogen sensor development:** Robert Bastasz and Josh Whaley confer in the Sandia/CA ion beam laboratory (2000)



**Tritium Plasma Experiment** developed at Sandia/CA: Rion Causey and Wayne Chrisman depicted with tritium TDS system (1993)

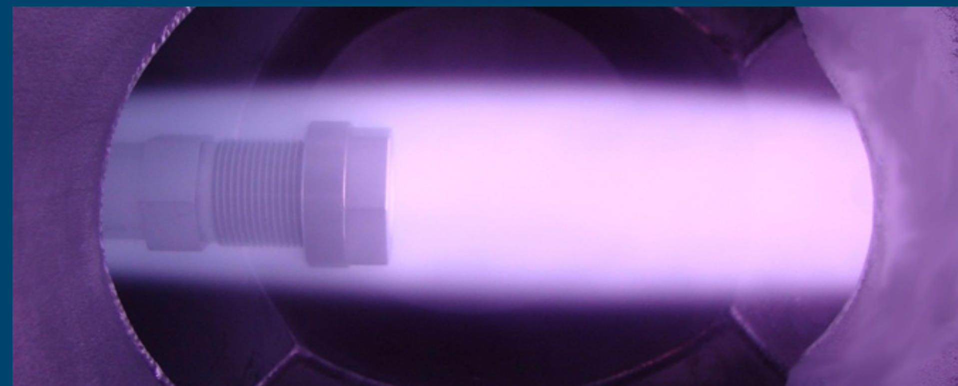
# Magnetic fusion research at Sandia/CA



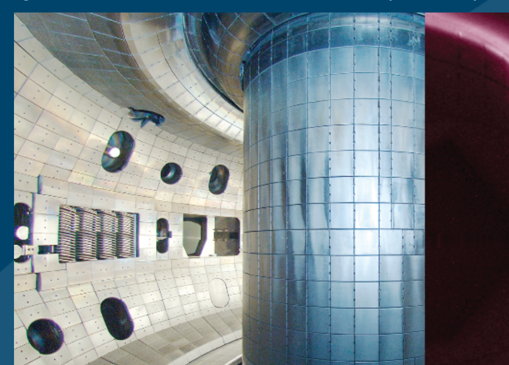
**Surface Effects:** H adsorption kinetics, composition of liquid metal surfaces (University of Tennessee, Princeton University, University of Illinois)

**H Micro-sensor Development** (DIII-D, PPPL)

**Tritium Retention / Permeation** (INL / PHENIX)



In-situ surface analysis / PSI Research
Edge Plasma Measurements (DIII-D)




DIII-D
NATIONAL FUSION FACILITY

# Underlying physics of plasma-material interactions

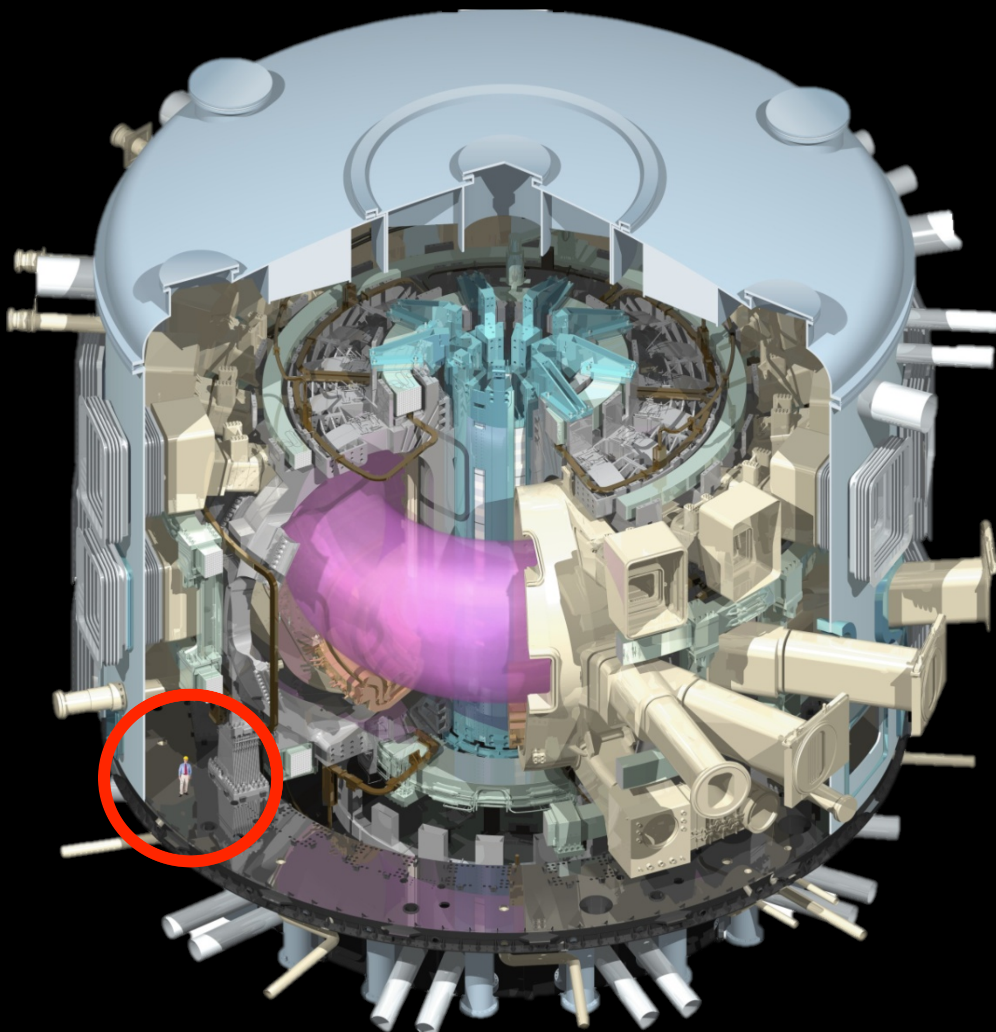
# Motivation: plasma-materials interactions for magnetic fusion

**ITER goals:**

- Achieve Q > 5 for D+T plasmas.
- Demonstrate technologies needed for power reactor

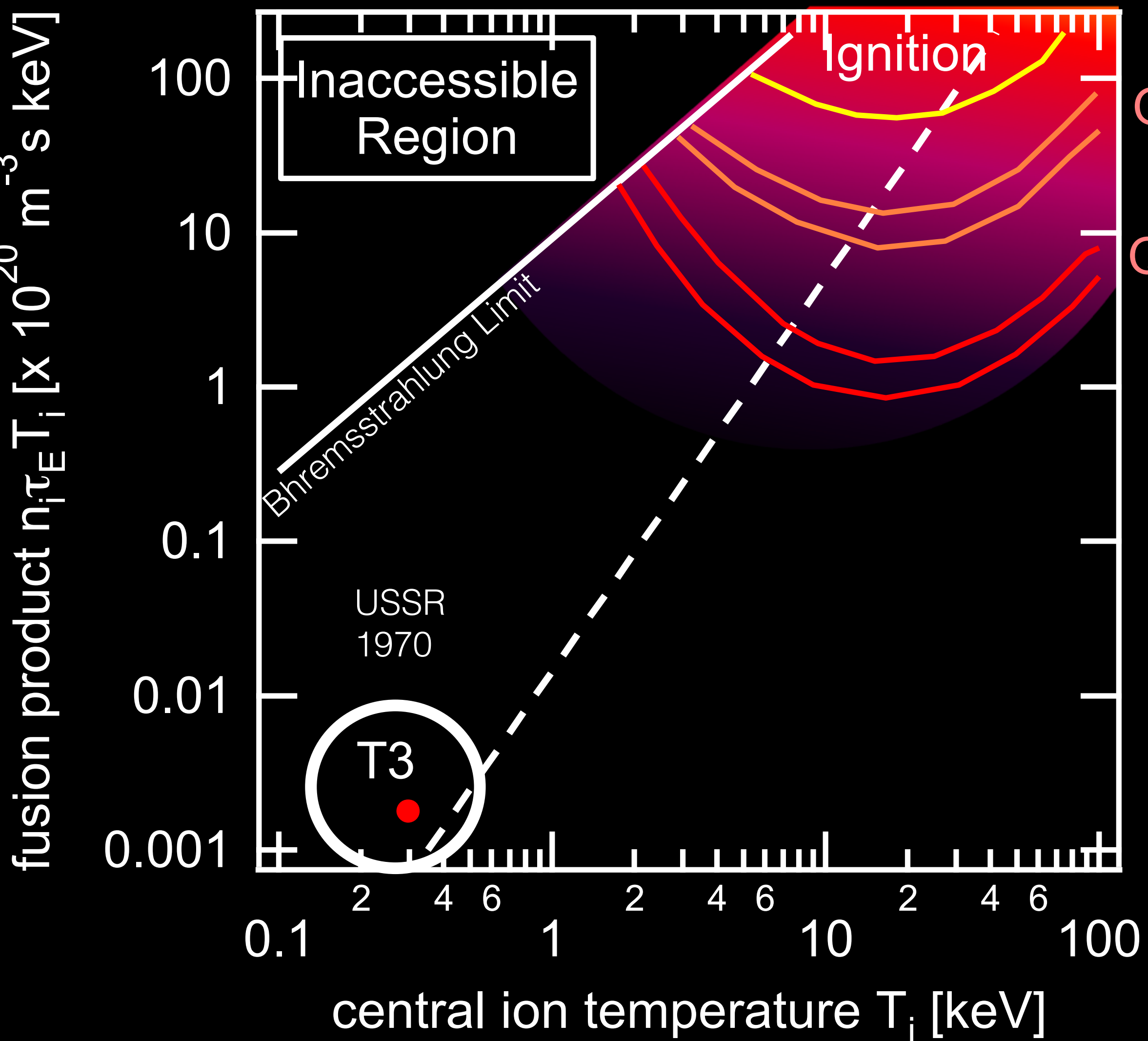
**Project details:**

- 7 Member Organizations
- Construction underway at Cadarache facility
- Expected first plasma: 2027
- Projected Cost: $20 B (45 % EU, 9% ea. from remaining partners.)



ITER

# Considerable progress in understanding of fusion plasmas over past decades




FIGURES OF MERIT:

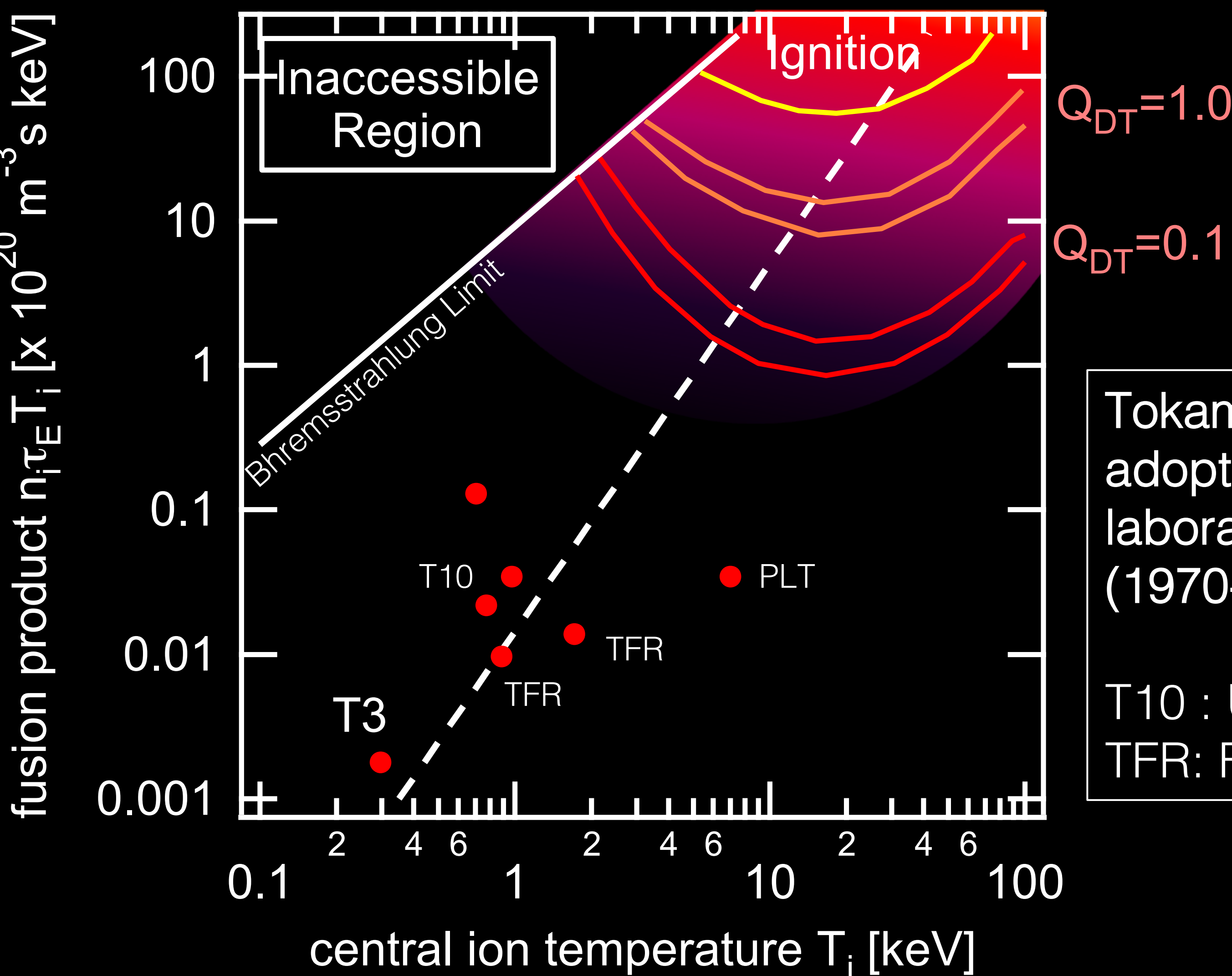
triple product: $n_i\tau_E T_i$

ion temperature: $T_i$

ENERGY MULTIPLICATION FACTOR:

$Q = P_{fusion}/P_{heating}$

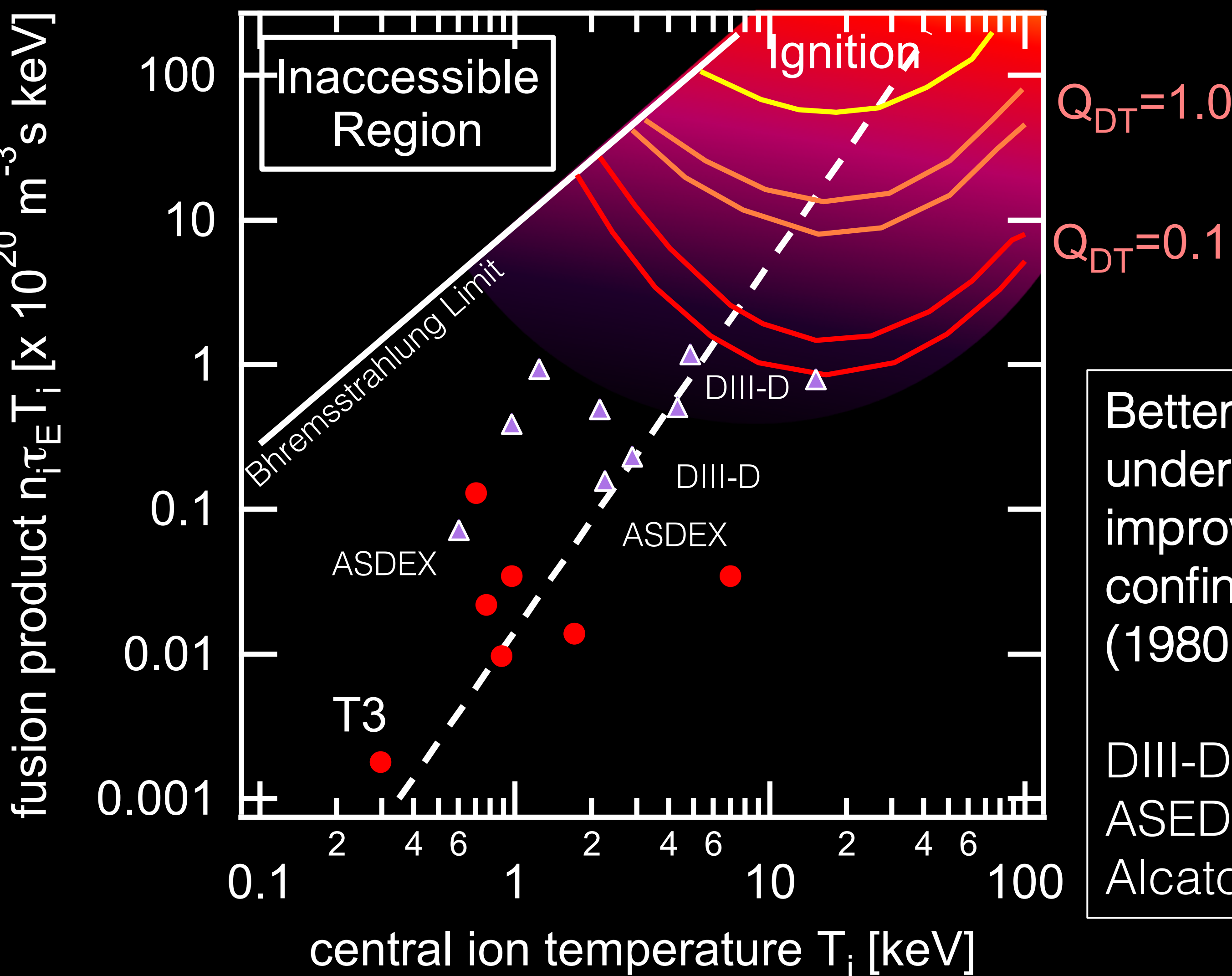
# Considerable progress in understanding of fusion plasmas over past decades




Tokamak design adopted by most major laboratories (1970-1980)

T10 : USSR
TFR: France

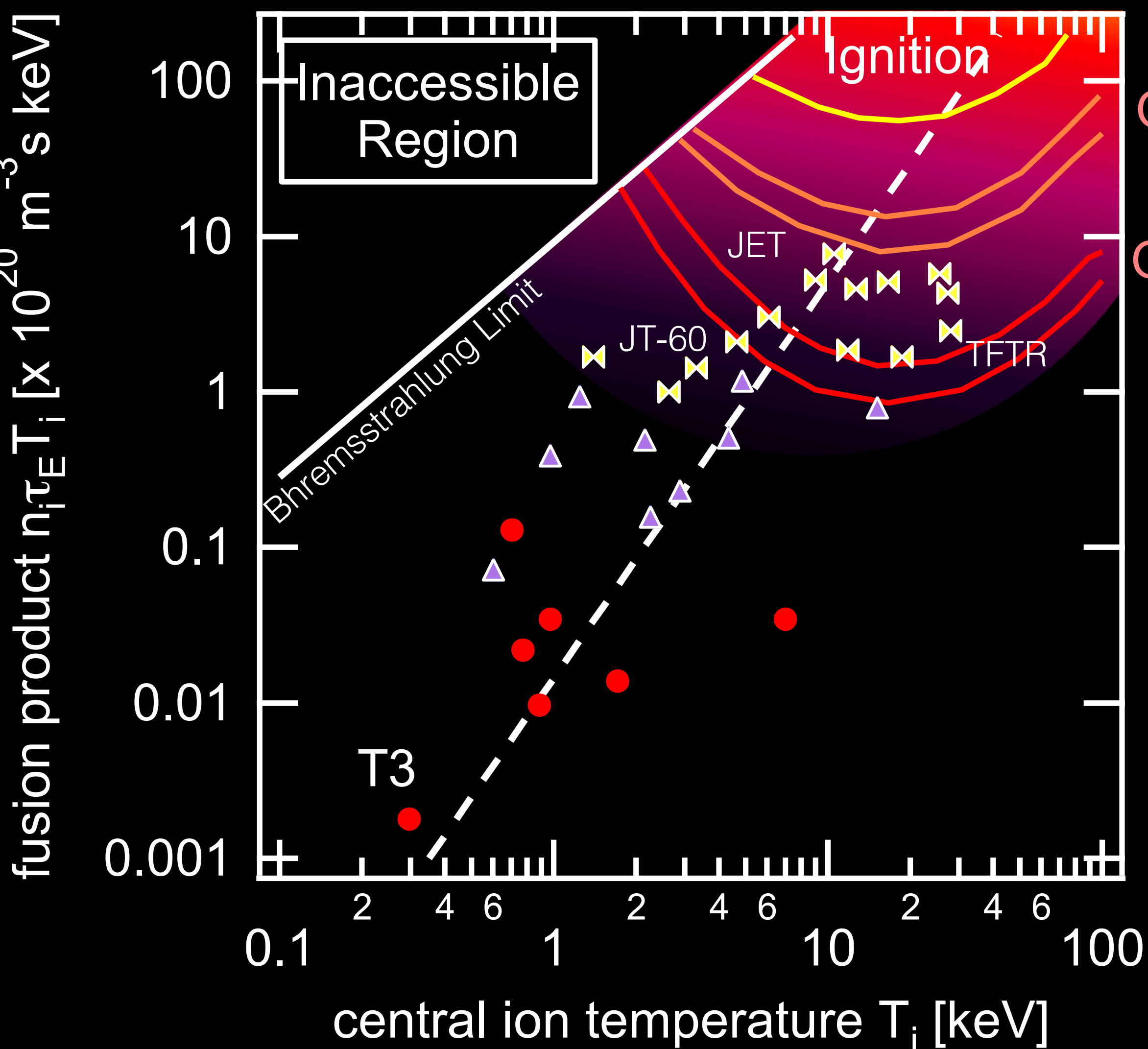
# Considerable progress in understanding of fusion plasmas over past decades




Better understanding of underlying physics improves plasma confinement [H-mode] (1980's)

DIII-D : USA
ASEDEX: Germany
Alcator C: USA

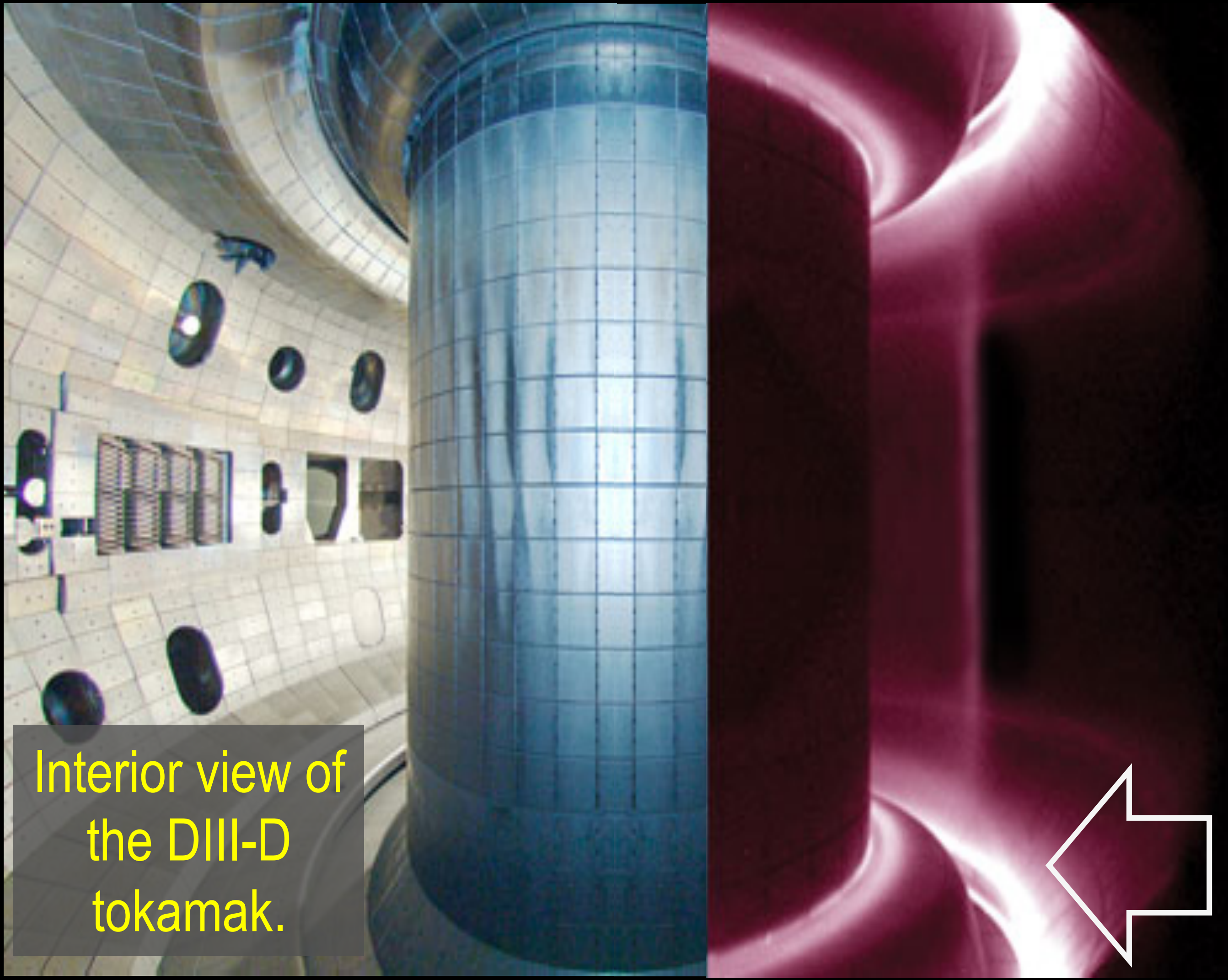
# Considerable progress in understanding of fusion plasmas over past decades




Large tokamaks achieve record density, confinement

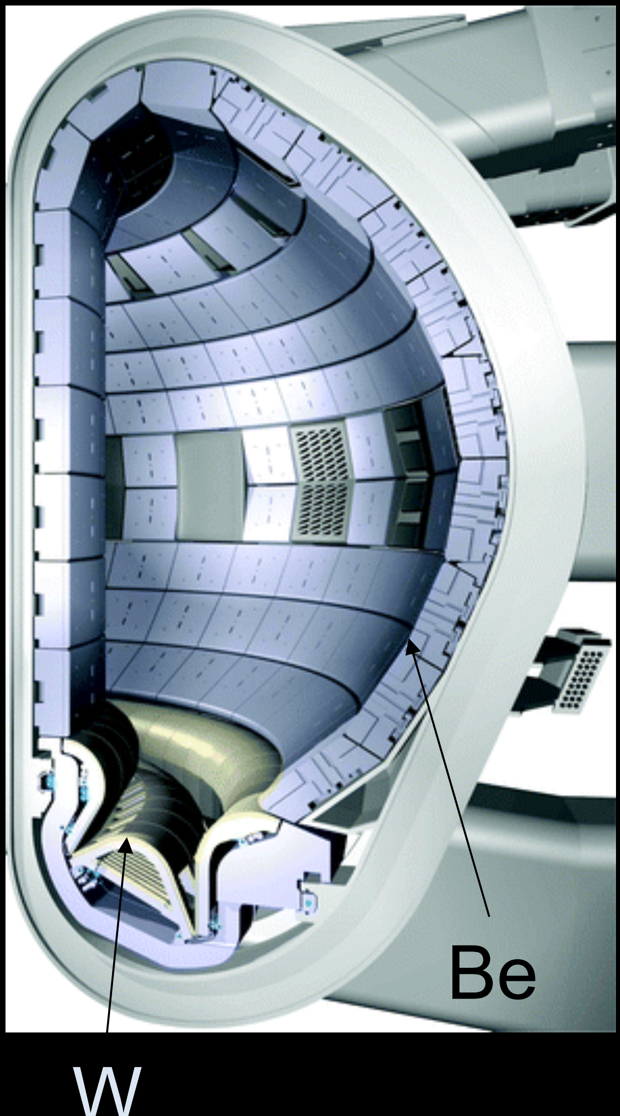
JET: EU
JT-60: Japan
TFTR: PPPL

# Primary challenges associated with fusion have increasingly focused on materials




Magnetic field lines diverted into secondary chamber where they interact with the wall to reduce impurities, known as the "divertor".

# Plasma exposure conditions are very demanding




**Exposure conditions:**

- High-flux D-T plasmas
- High-energy fusion products (14 MeV n, helium ash)
- Impurities
- High transient heat and particle loads

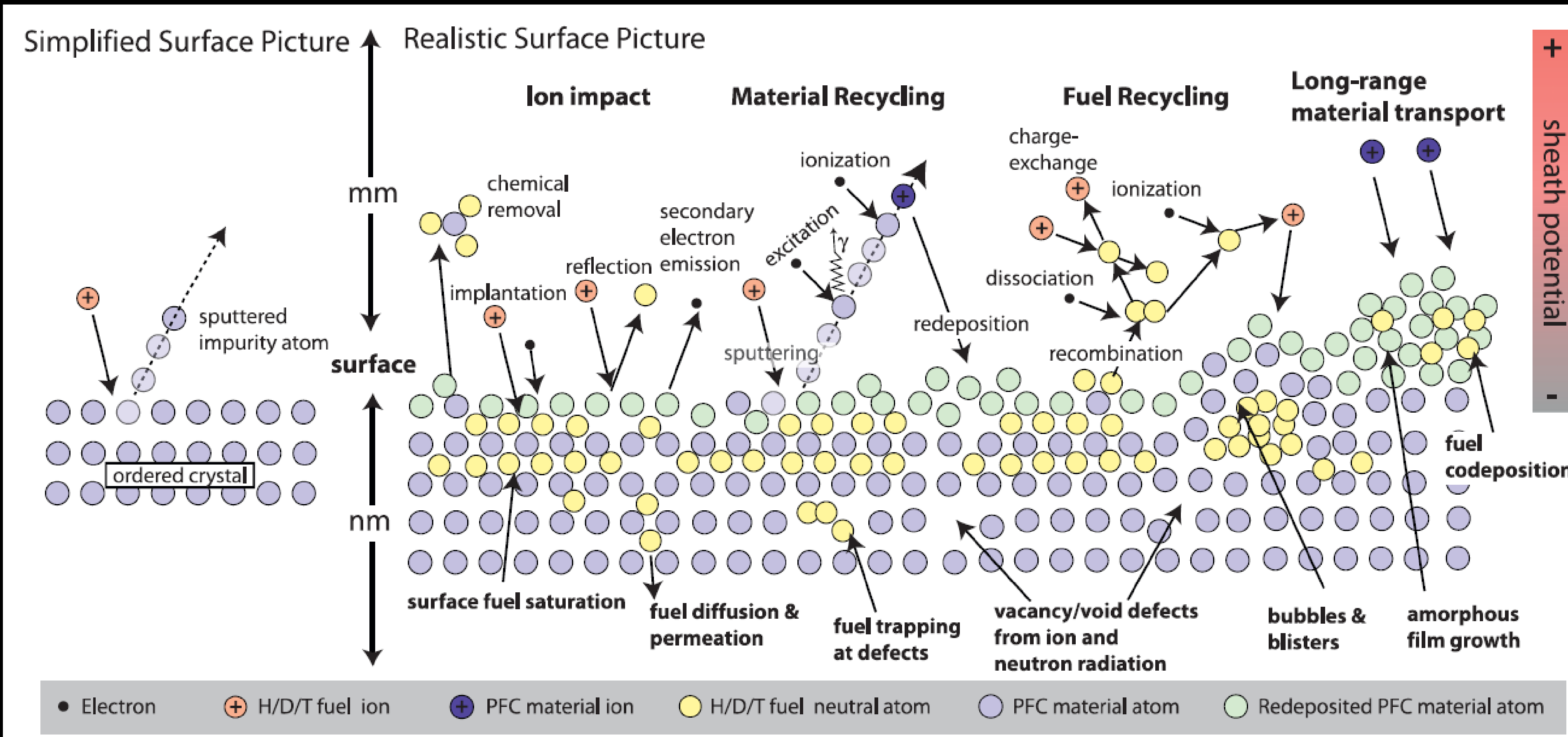
**Relevant Materials:**

DIII-D: C; NSTX: Mo, C, Li

ITER: Be & W

DEMO: Advanced W or liquid metals

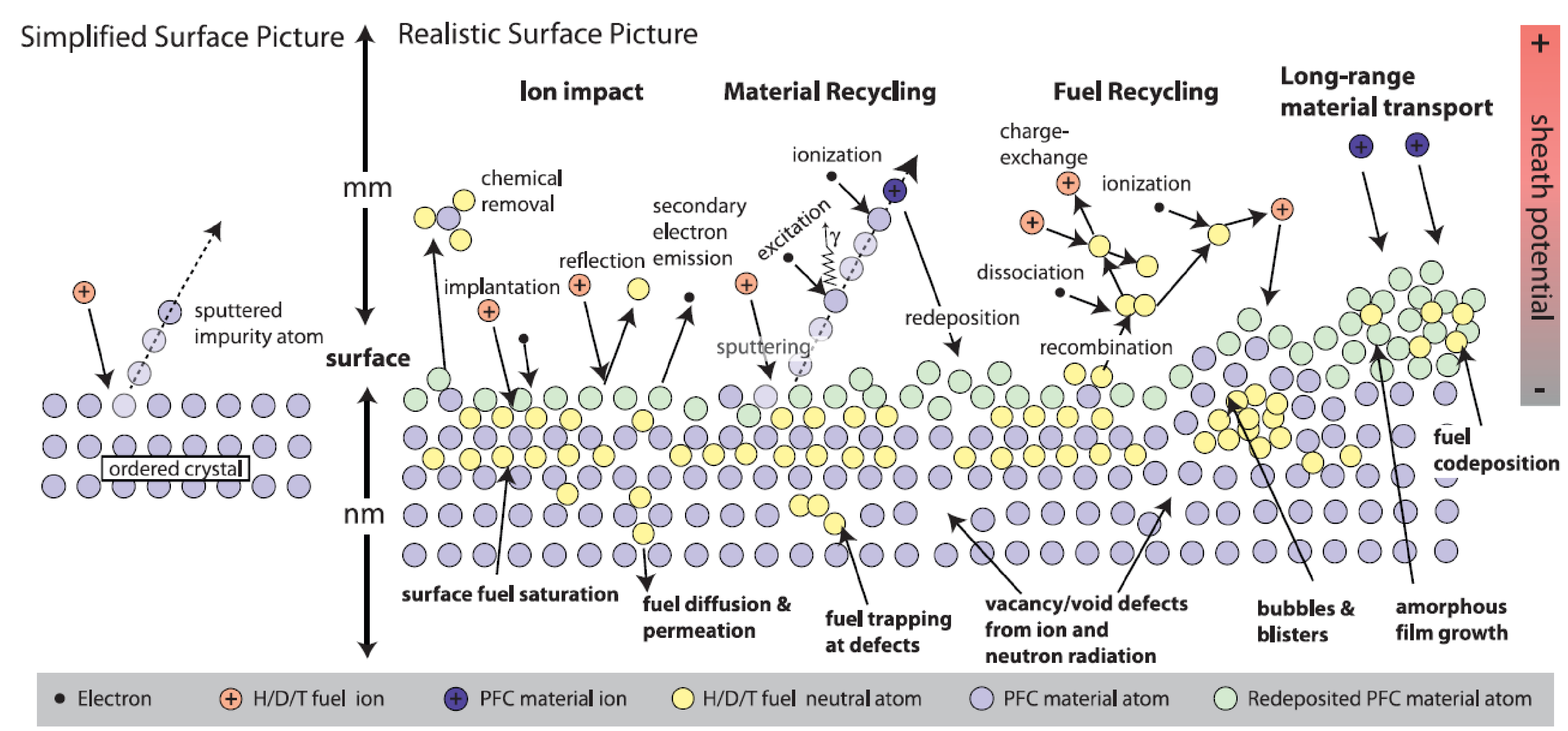
# Relevant processes span many orders of magnitude in length and time scales




- Many simultaneous processes
- Relevant length and time scales span several orders of magnitude

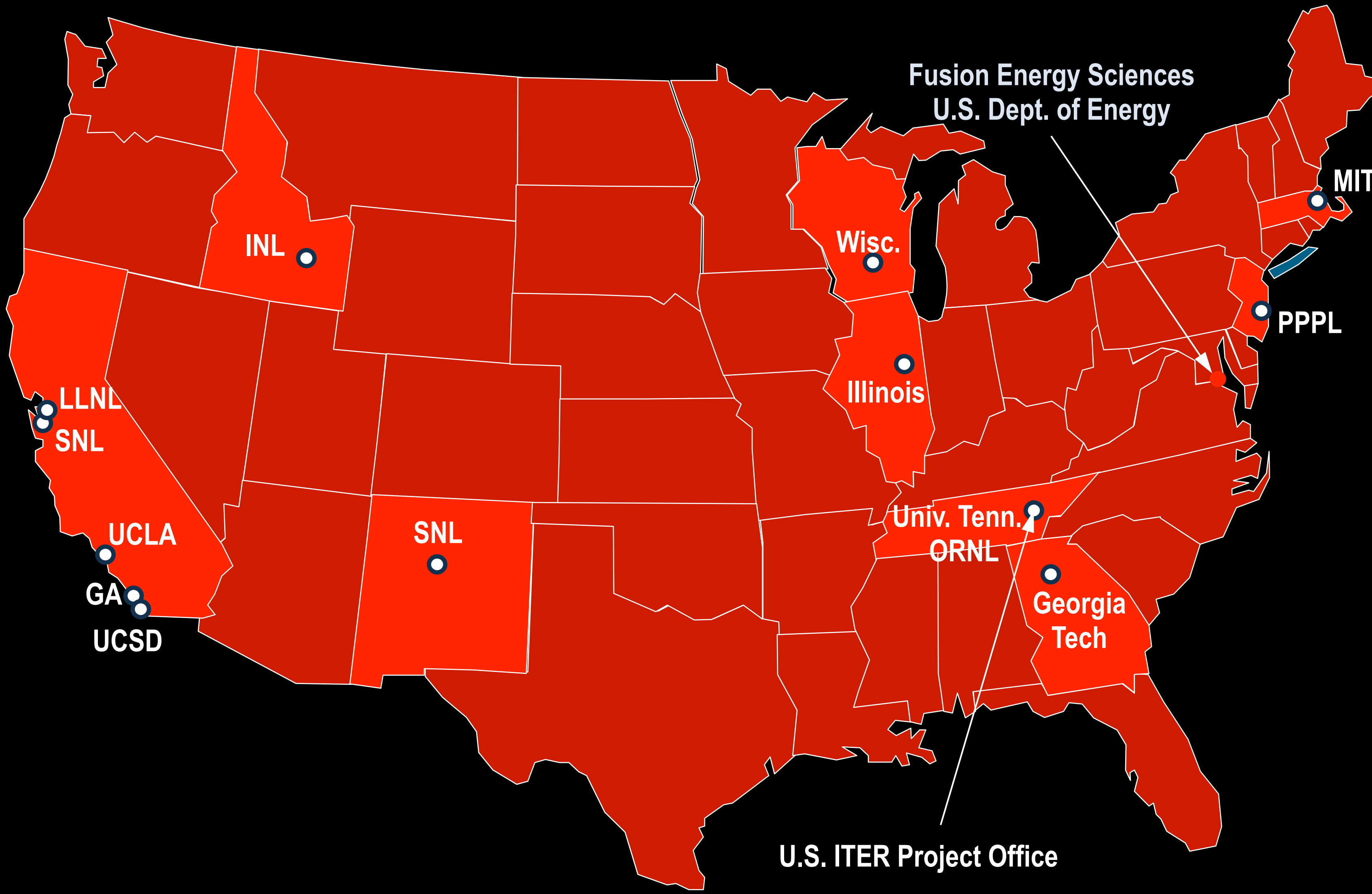
Image from: B. D. Wirth, K. Nordlund, D. G. Whyte, and D. Xu, *MRS Bull.* **36** (2011) 216

# Relevant processes span many orders of magnitude in length and time scales

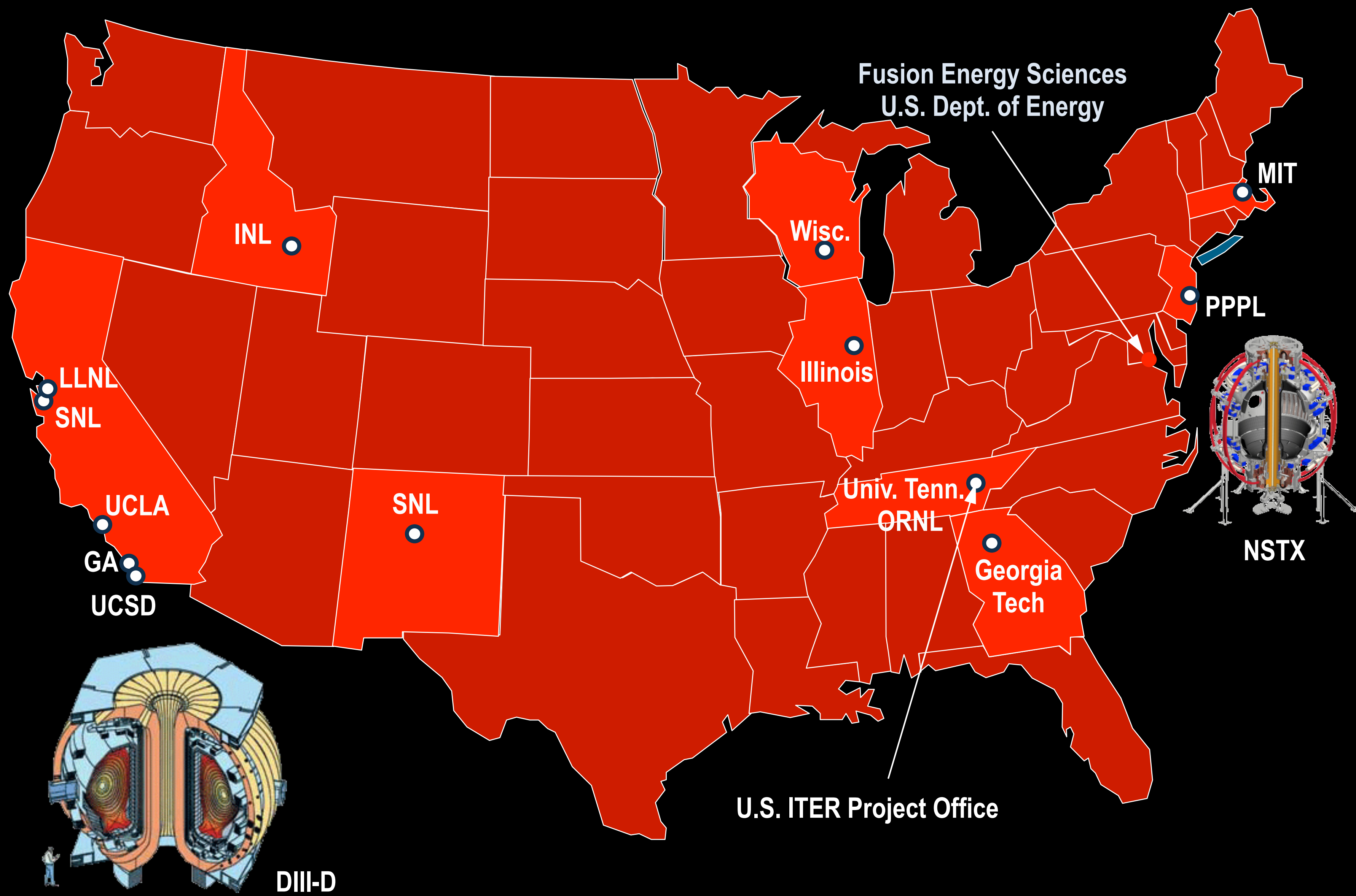



- What experiments would enable us to decipher the complex physics occurring at the surface?
- Can we model how the surfaces evolve with plasma exposure?

# Principal U.S. sites with PMI Activities

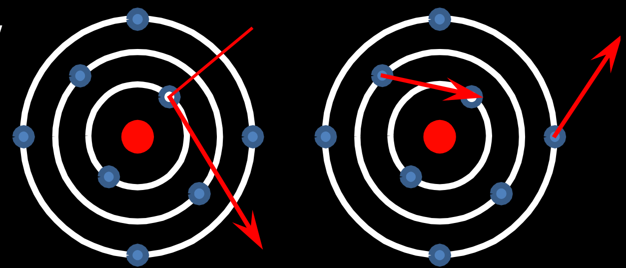


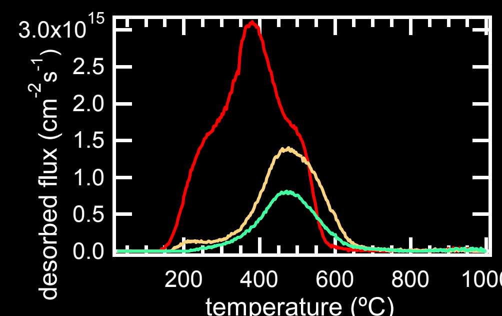
# Principal U.S. sites with PMI Activities



# Fundamental changes to surface chemistry & structure derived from surface analysis techniques

Auger Electron Spectroscopy



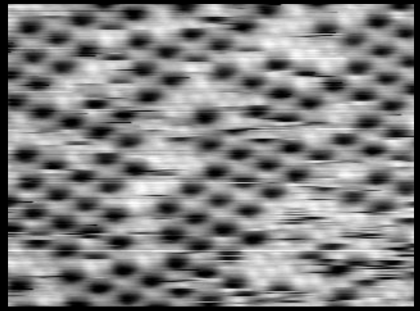


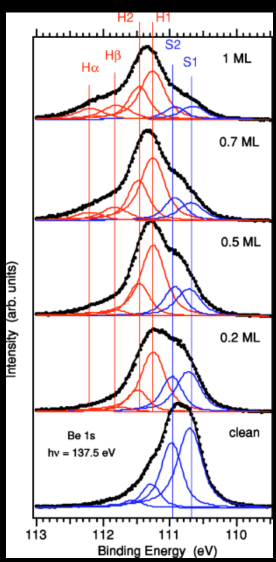

Thermal desorption spectroscopy

**"Single effect" devices enable us to isolate specific physical processes**

- Examine response of surfaces to well-controlled exposure conditions
- Involve the use of simplified material geometries (e.g. single crystals)

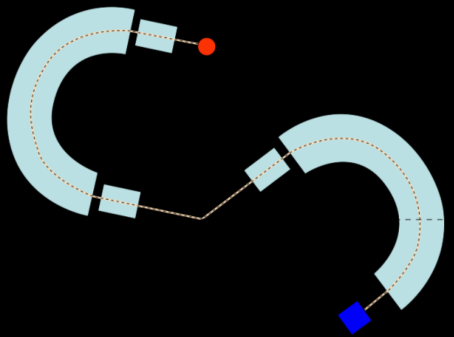
Scanning tunneling microscopy






X-ray photoelectron spectroscopy

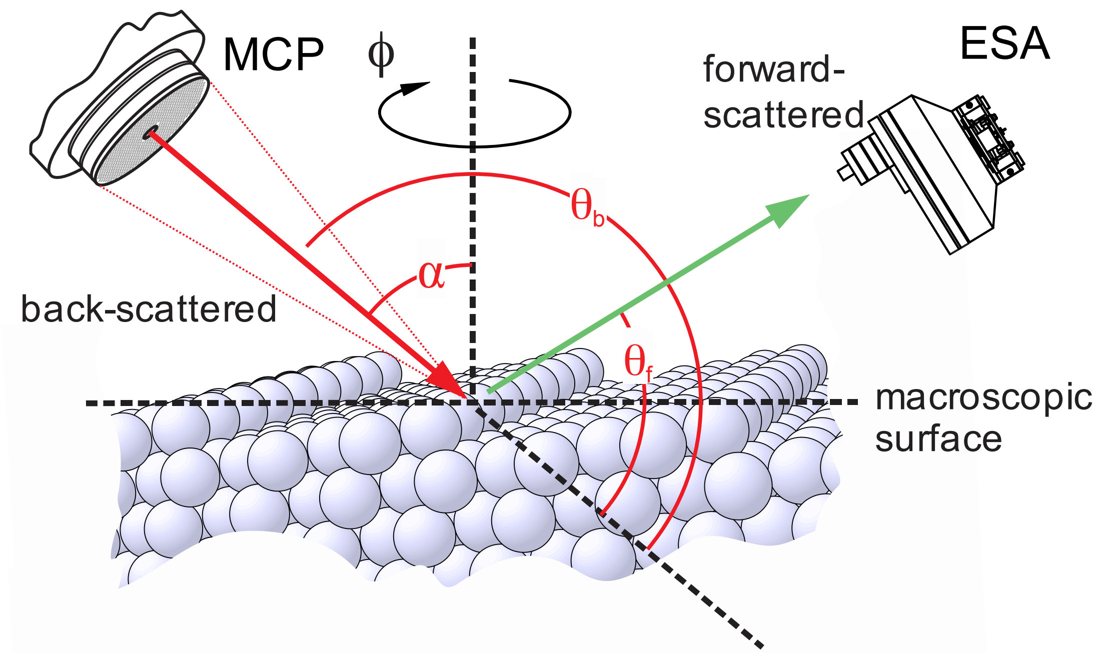
Low energy electron diffraction

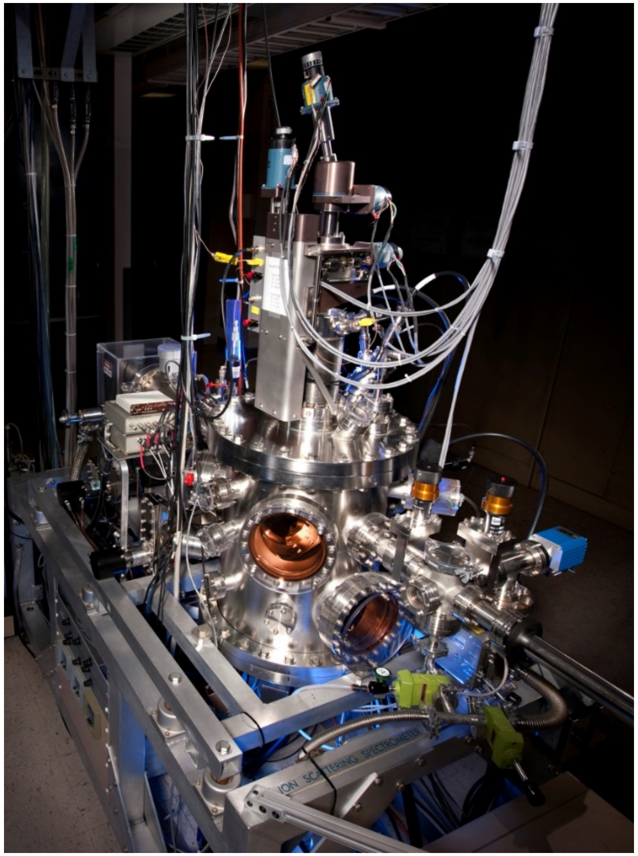


High-resolution electron energy loss spectroscopy

# Example: use of ion energy spectrometer to study hydrogen chemisorption

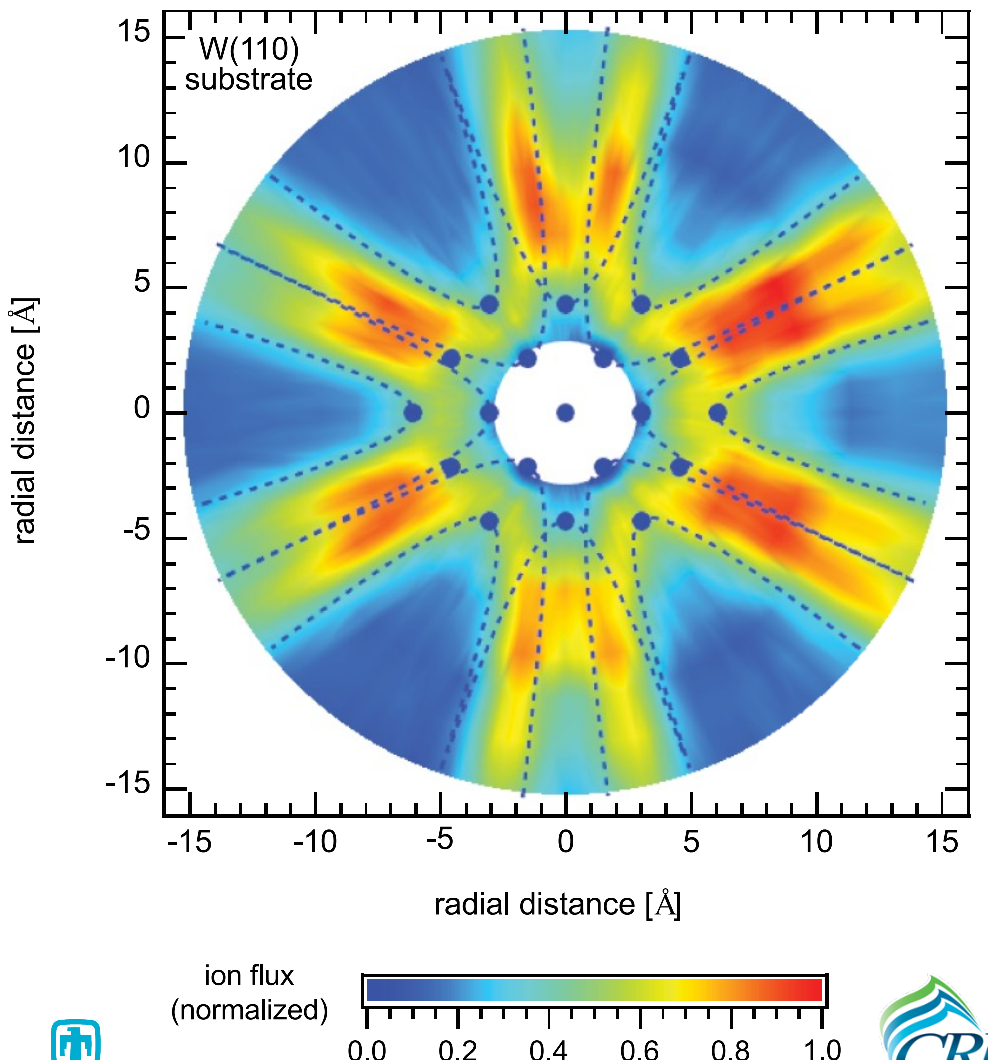
**Angle-resolved ion energy spectrometer**



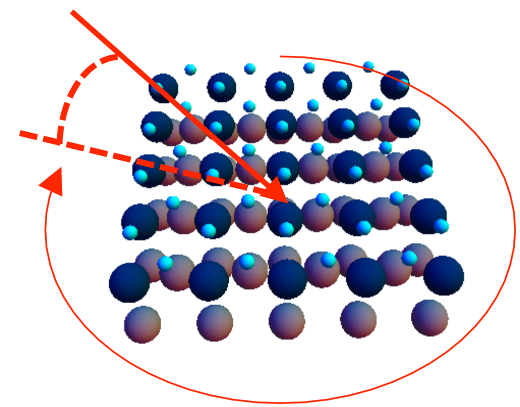



- Mass-separated beam (< 5 keV $He^+$, $Ne^+$)
- Tungsten capillary for atomic hydrogen dosing.
- Load-lock / clean transfer system available for air-sensitive samples

# W(110) substrate configuration determined from large angle scattering map

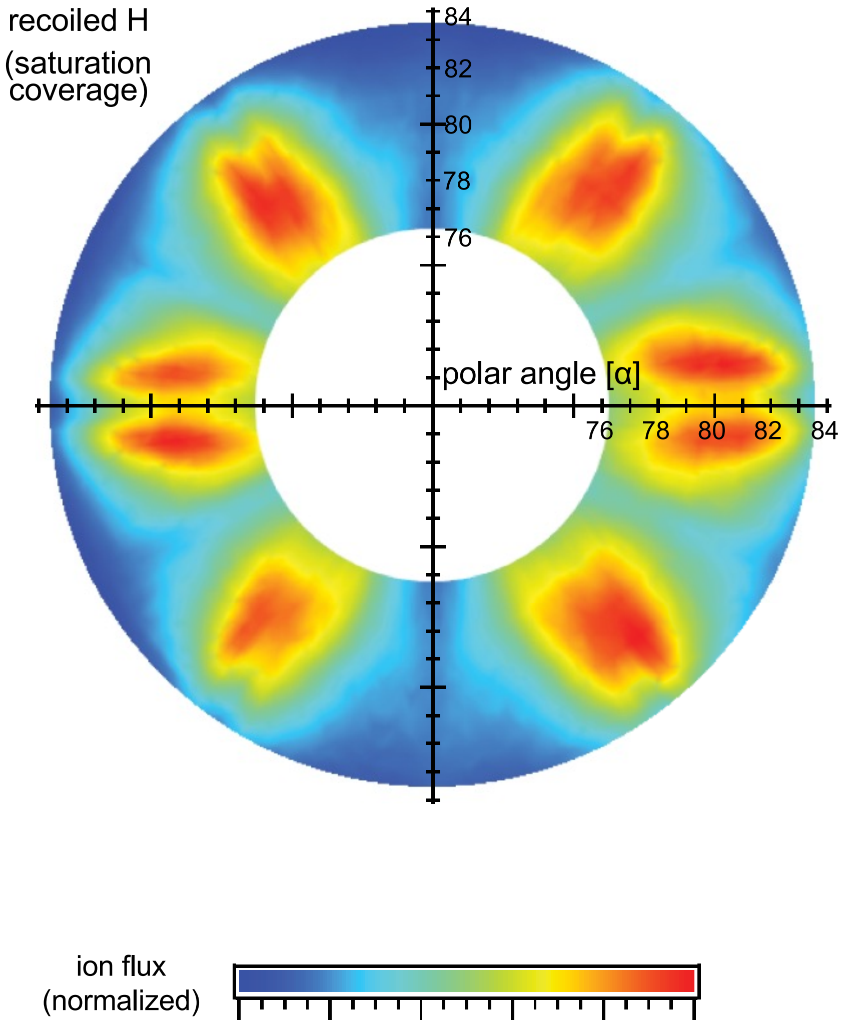


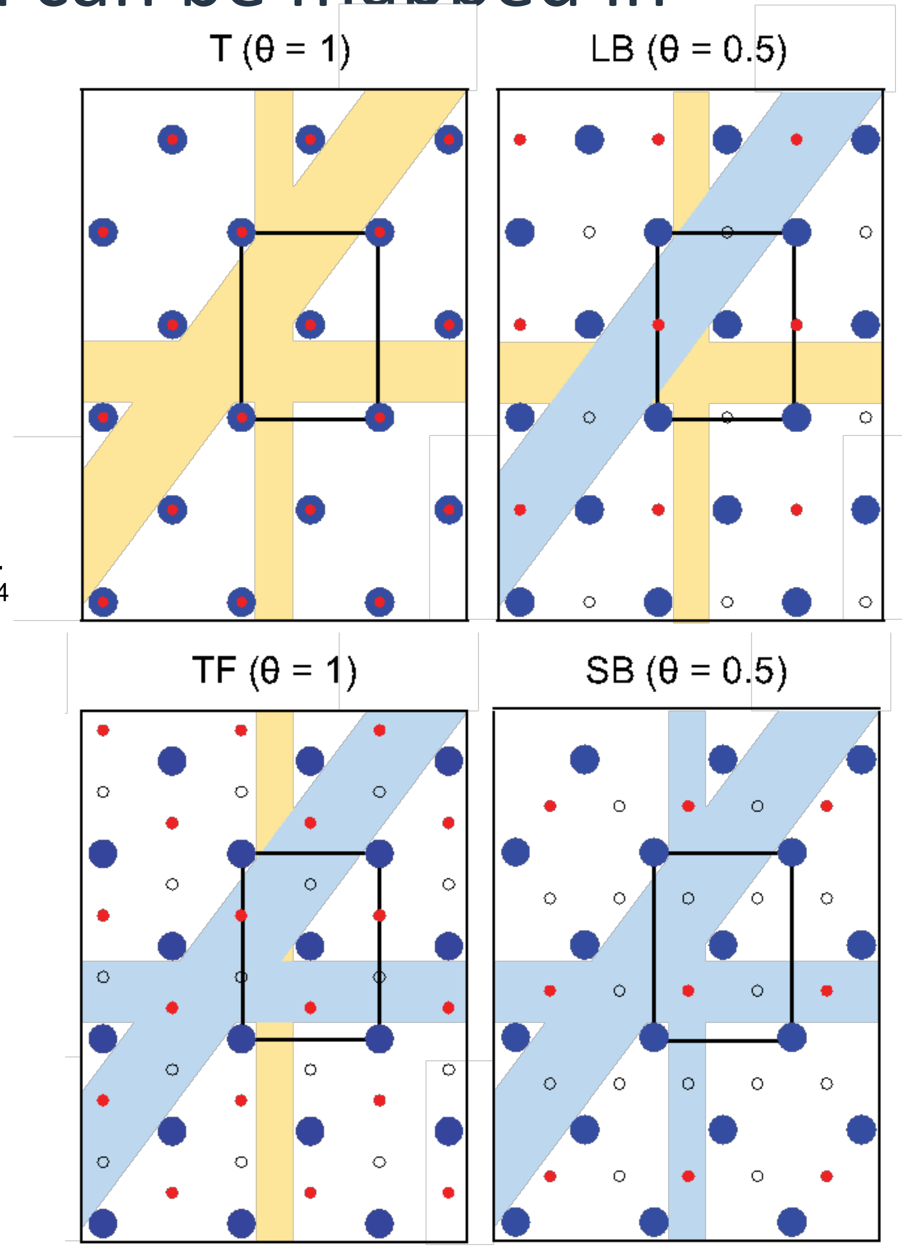

Map created by varying 1 keV $Ne^{+}$ incidence angle and crystal azimuth.



- Scattering pattern consistent with non-reconstructed, clean surface.
- W atoms are effective at deflecting $Ne^{+}$ along open surface channels.

# Chemisorbed hydrogen can be mapped in the same manner



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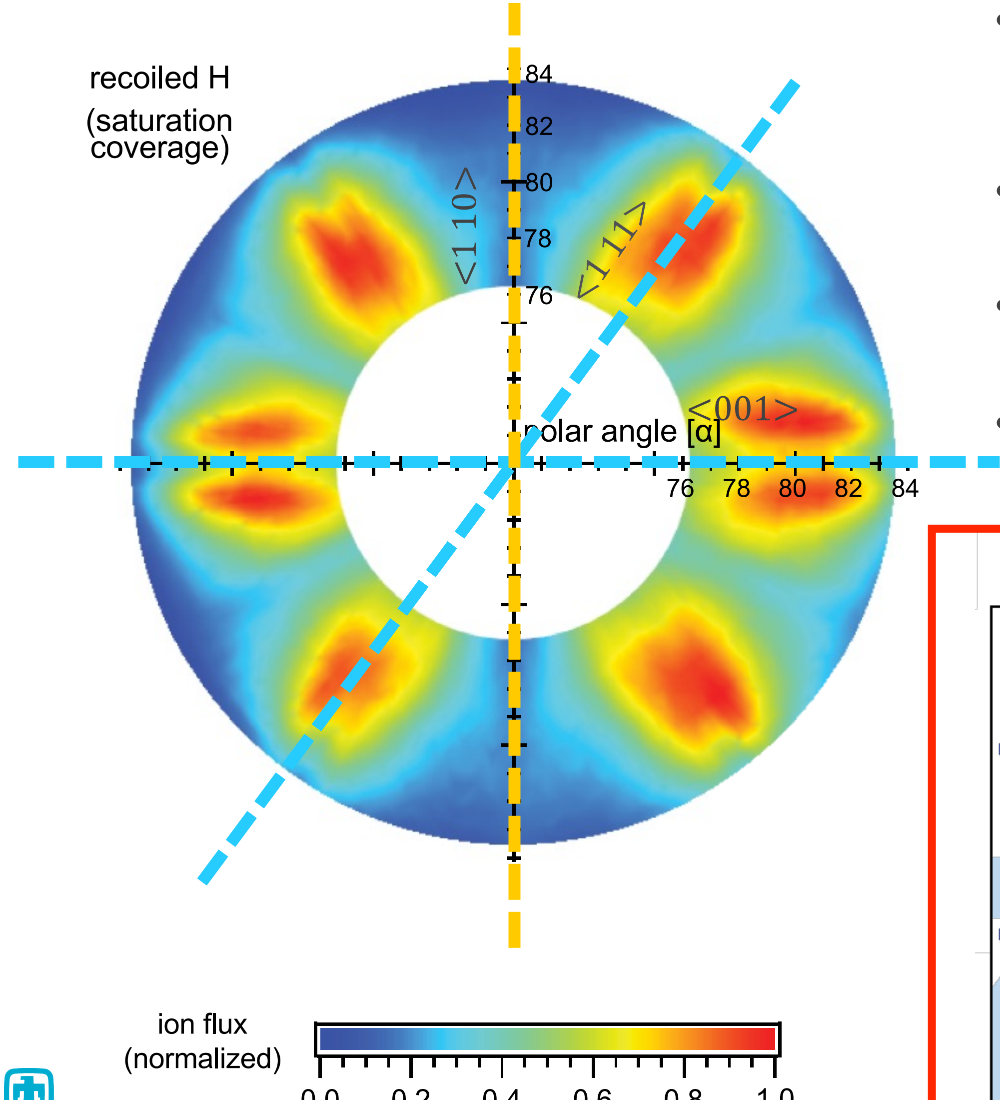
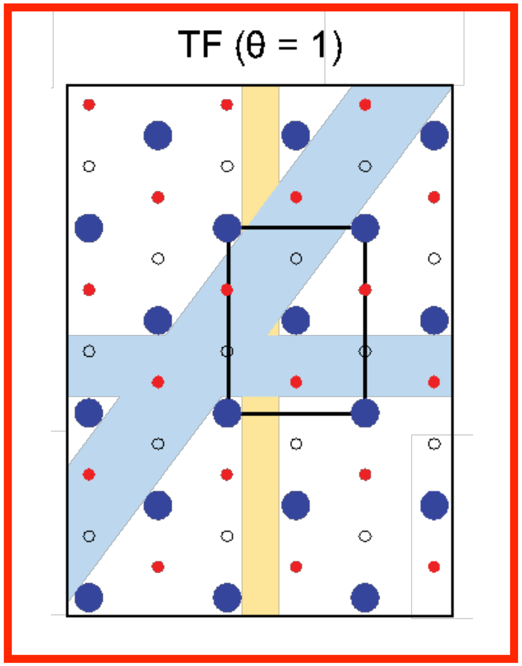



- Hydrogen readily chemisorbs on W(110) surface without a dissociation barrier.
- Recoiled hydrogen observed along <001> and <1 11> channels
- No recoils observed along <1 10> channels.
- Consistent with binding to three fold hollow sites.



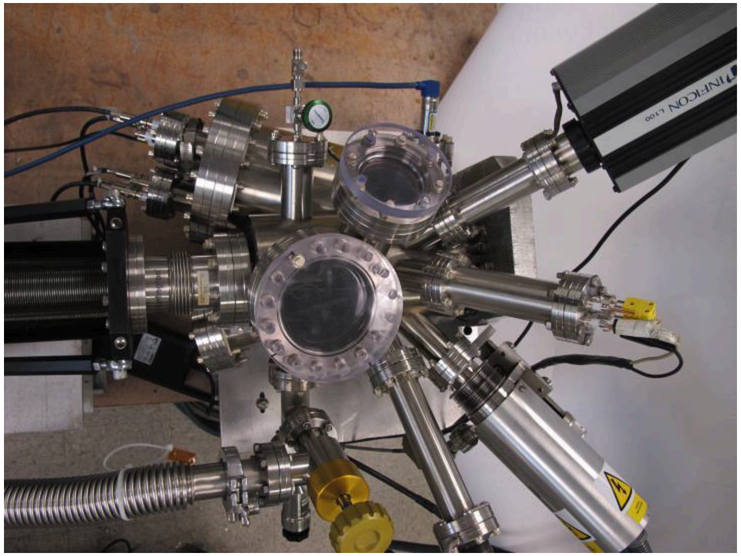
# Confinement device-based exposure platforms: In-situ PMI studies in LTX / NSTX-U

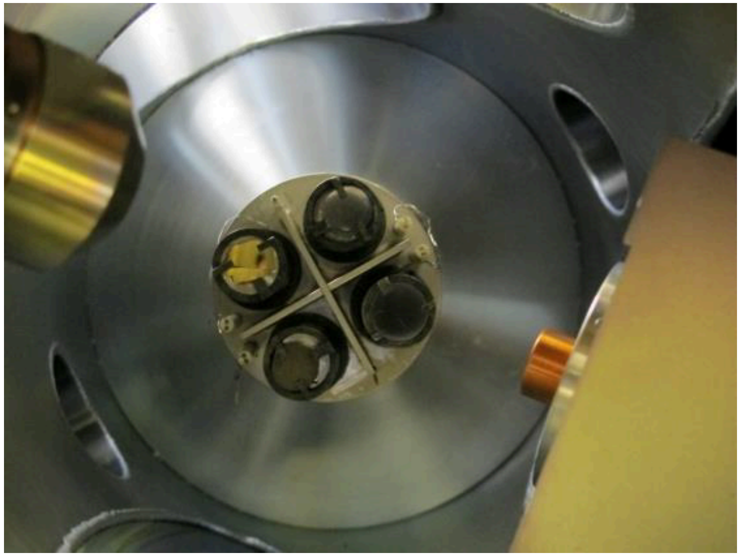
**Materials Analysis and Particle Probe (MAPP)**

- In-vacuum PMI diagnostic to determine material composition and surface chemistry
- Up to 4 samples can be exposed to divertor plasma

**Diagnostics**

- X-ray photo electron spectroscopy
- Low energy ion scattering
- Thermal desorption spectrometry





# Confinement device-based exposure platforms: DiMES / MiMES on DIII-D


DiMES

MiMES

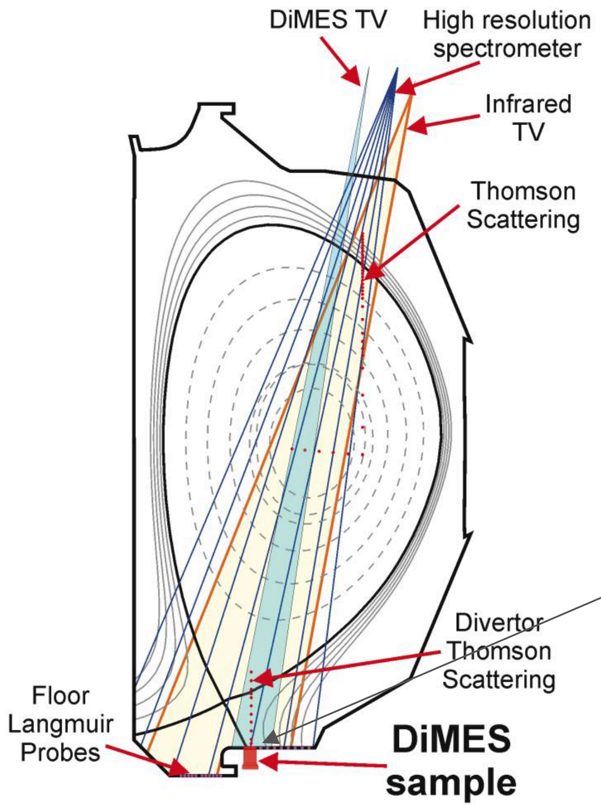
**In-situ exposure platform for PMI studies**

- Erosion measurements carried out via post-mortem RBS
- Can also be used as a means of inserting probes into the plasma

**Recent work includes:**

- Studies of local erosion / redeposition
- In-situ beta backscattering to map metal contamination on graphite tiles
- Support of metal ring campaign

# Work with DiMES is an example of the collaborative nature of PMI research in the U.S.




Supported by **DIII-D** Diagnostic Group and technical staff

**SNL-L** Sample preparation and diagnostics development (Langmuir probe)

**SNL-NM** Surface analysis after exposure (RBS)

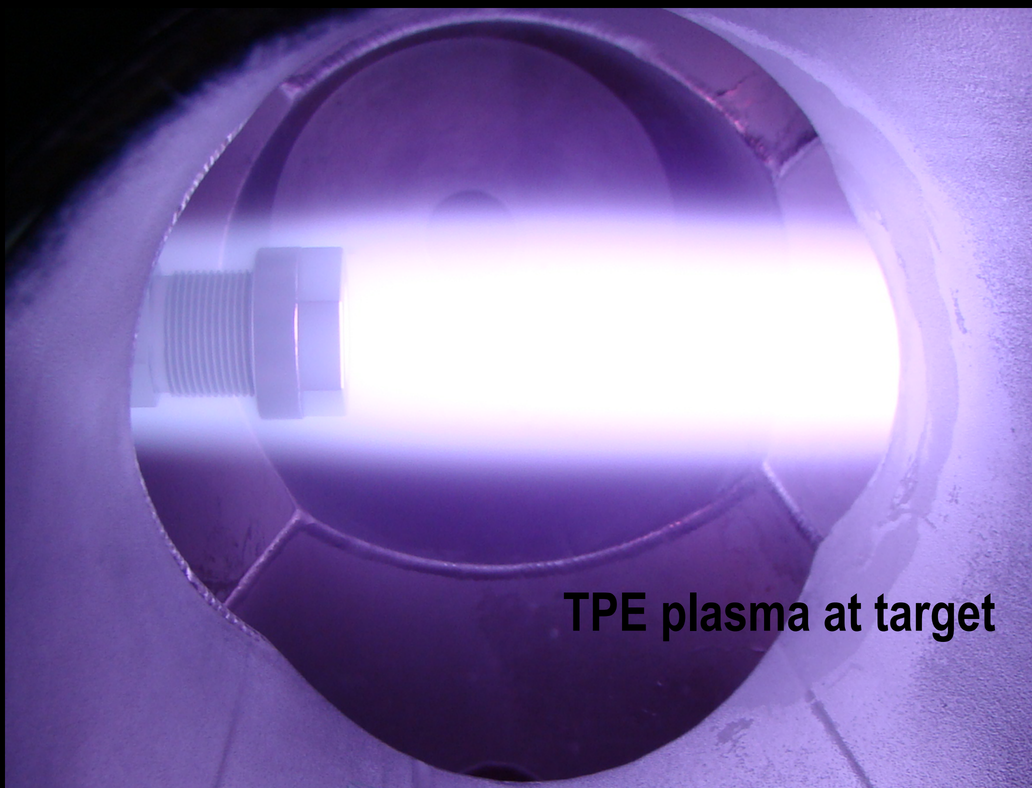
**U of Toronto** Edge physics and modeling

**U Tenn / ORNL** Surface analysis (ICPMS)

**GA** – Chemistry and surface analysis (SEM, EDX)

**UCSD** – Sample preparation

# Tritium migration and retention: use of "multi-effect" linear plasma devices




**Tritium Plasma Experiment**

Creates a well-defined plasma column, flux is approx. 1 A / $cm^2$

Simulates the plasma-flux conditions encountered in tokamaks in a highly-controlled manner.

Highest flux D+T linear plasma generator world-wide

# Working with tritium is … fun?

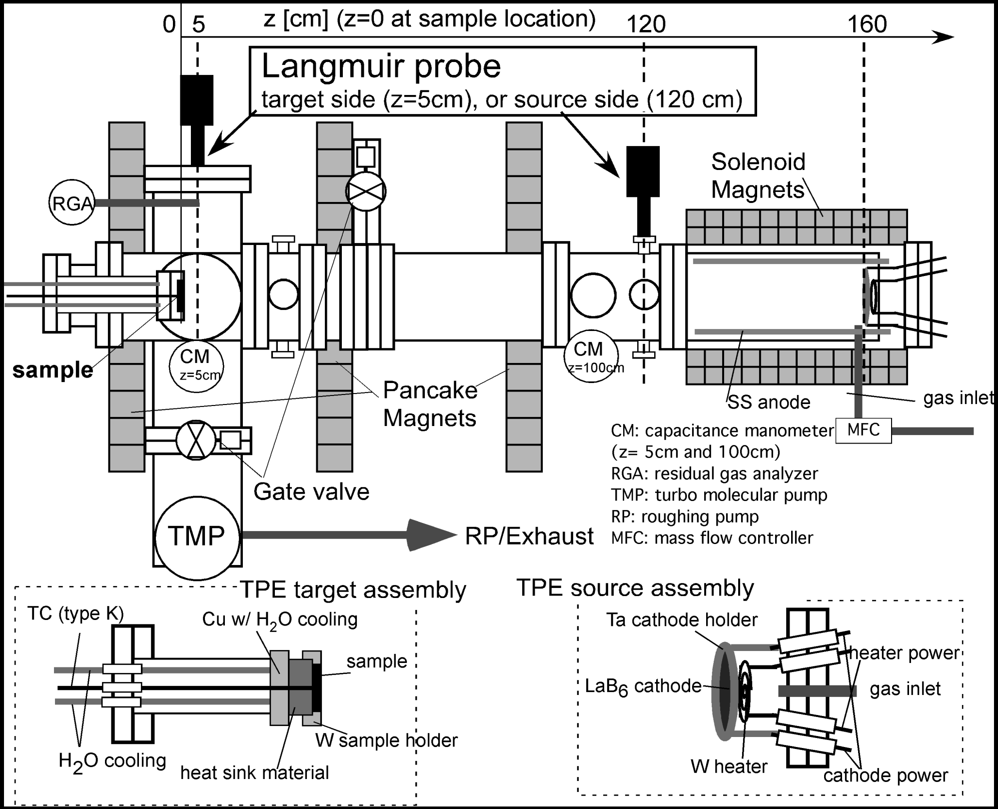

**Unique capabilities:**

- neutron-activated materials
- beryllium
- tritium imaging plate

**Tritium Plasma Experiment**

- Idaho National Laboratory and Sandia/CA collaboration
- Maximum facility inventory: 1.5 g (15000 Ci)
- Typical use: < 100 mCi per plasma exposure
- Provides 100 x sensitivity improvement

# Working with tritium is … fun?

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**Tritium Plasma Experiment**

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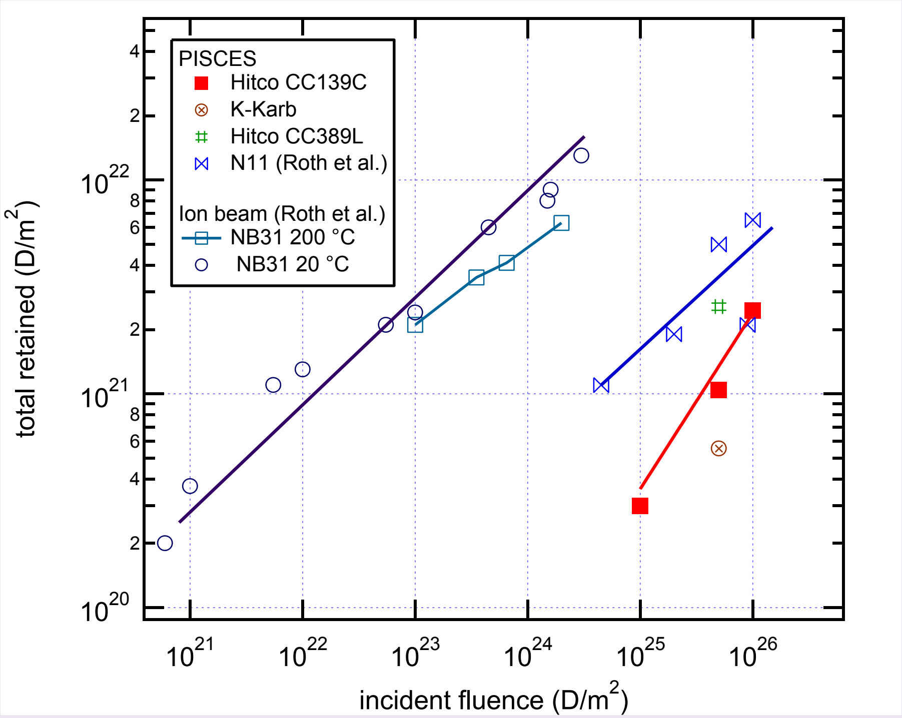
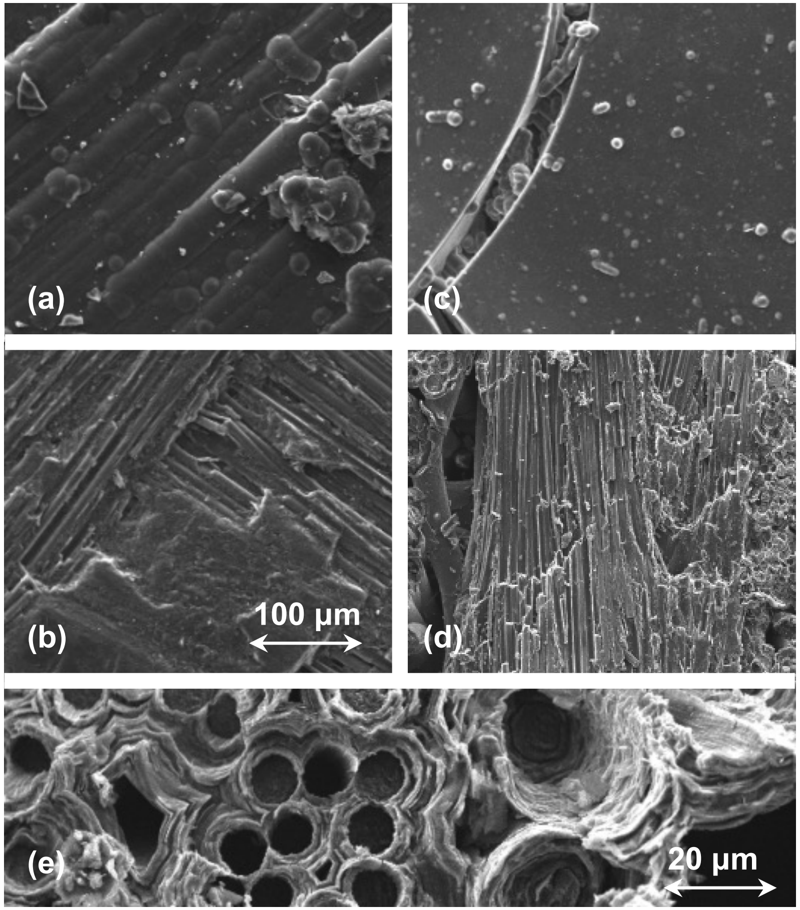
# CFC materials perform poorly from a tritium inventory standpoint

- High BET surface area for 3D CFC weave used in Tore Supra
- High surface porosity → high retention.
- Tritium rich co-deposits



# Diffusion and trapping modeled in tungsten with continuum-scale approach

## Diffusion

1-D diffusion, uniform temperature.

$$\partial u(x,t)/\partial t = D(t)\,\partial^2 u(x,t)/\partial x^2 - q_T(x,t) - q_B(x,t)$$

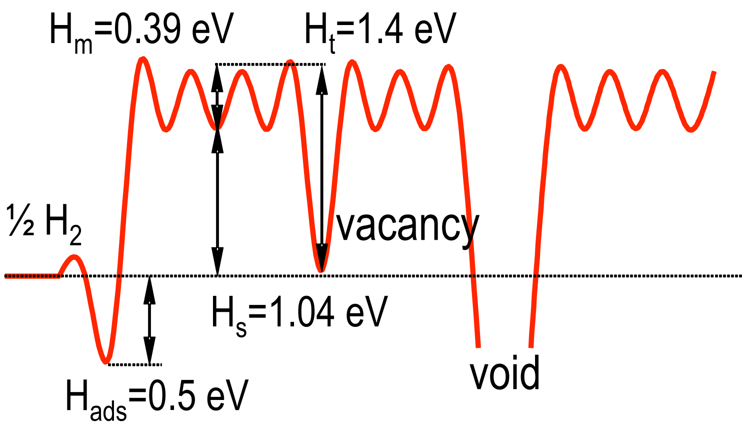
## Point defects

1.4 eV saturable traps, no nucleation. Approach of Ogorodnikova [*J. Nucl. Mater.* 2009] used for trapping and release.

## Bubbles:

Modeled using a simple approach developed by Mills [J. Appl. Phys. (1959)].

$$q_B = \partial u_B(x,t)/\partial t = 4\pi D(t) r_B(x,t) N_B(x)\left[u(x,t) - u_{eq}(x,t)\right]$$

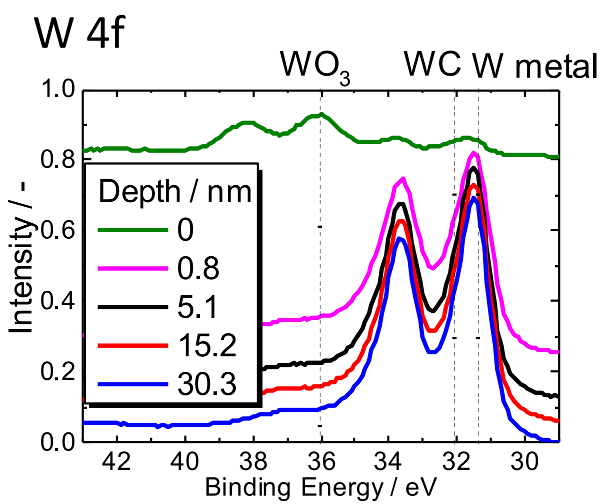



Energy diagram for H migrating through tungsten.

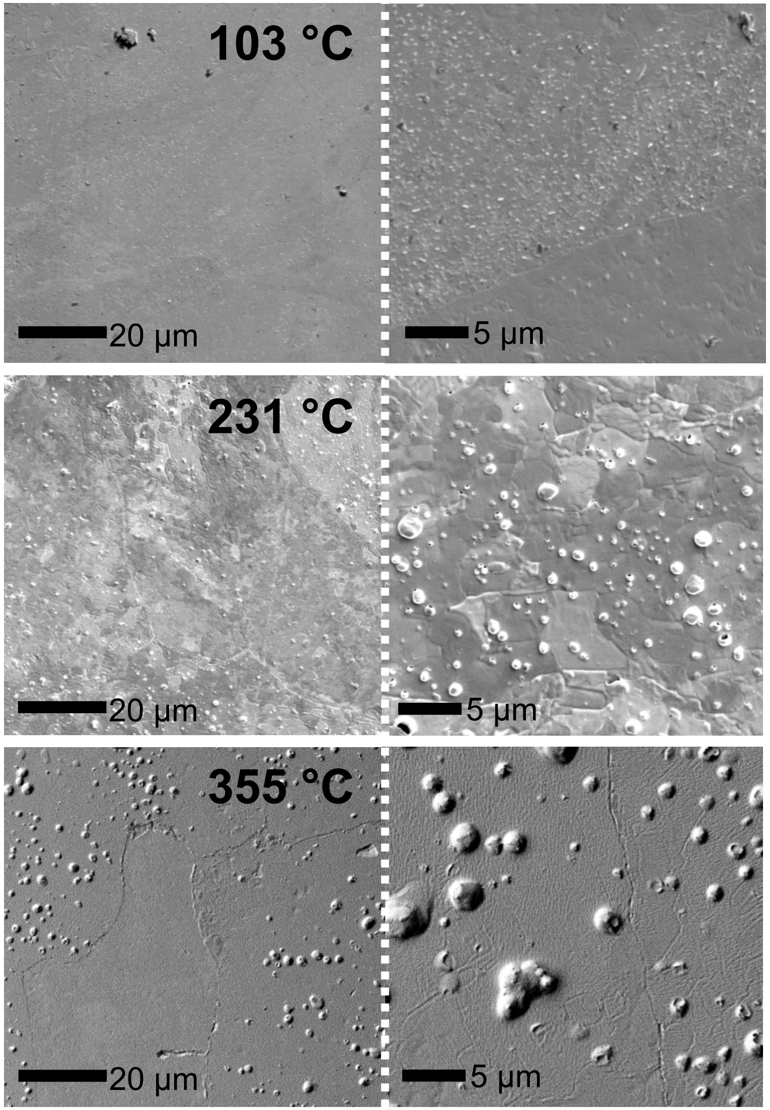
Dissolution of H in W is highly endothermic.

# Near-surface formation of H-filled bubbles leads to surface degradation

- Microscopy reveals near-surface H precipitates
- Density/size temp. dependence
- Growth determined by grain orientation

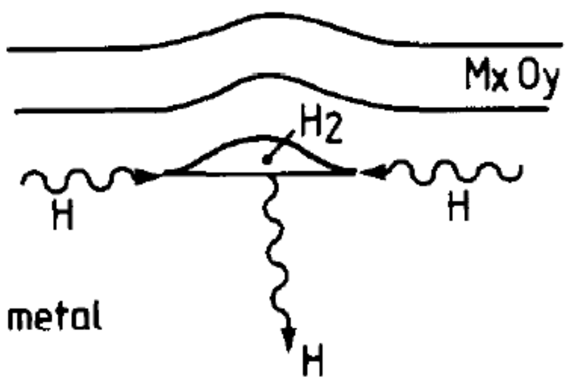



XPS reveals negligible WC

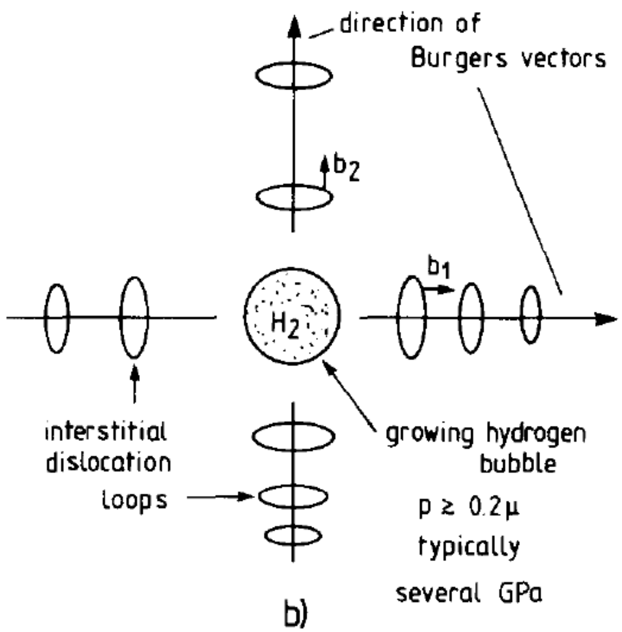


# How do near-surface bubbles grow?

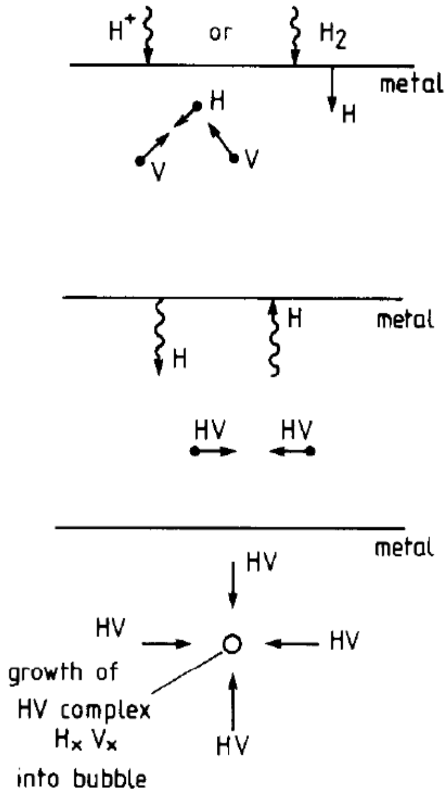
near-surface plastic deformation




dislocation loop punching



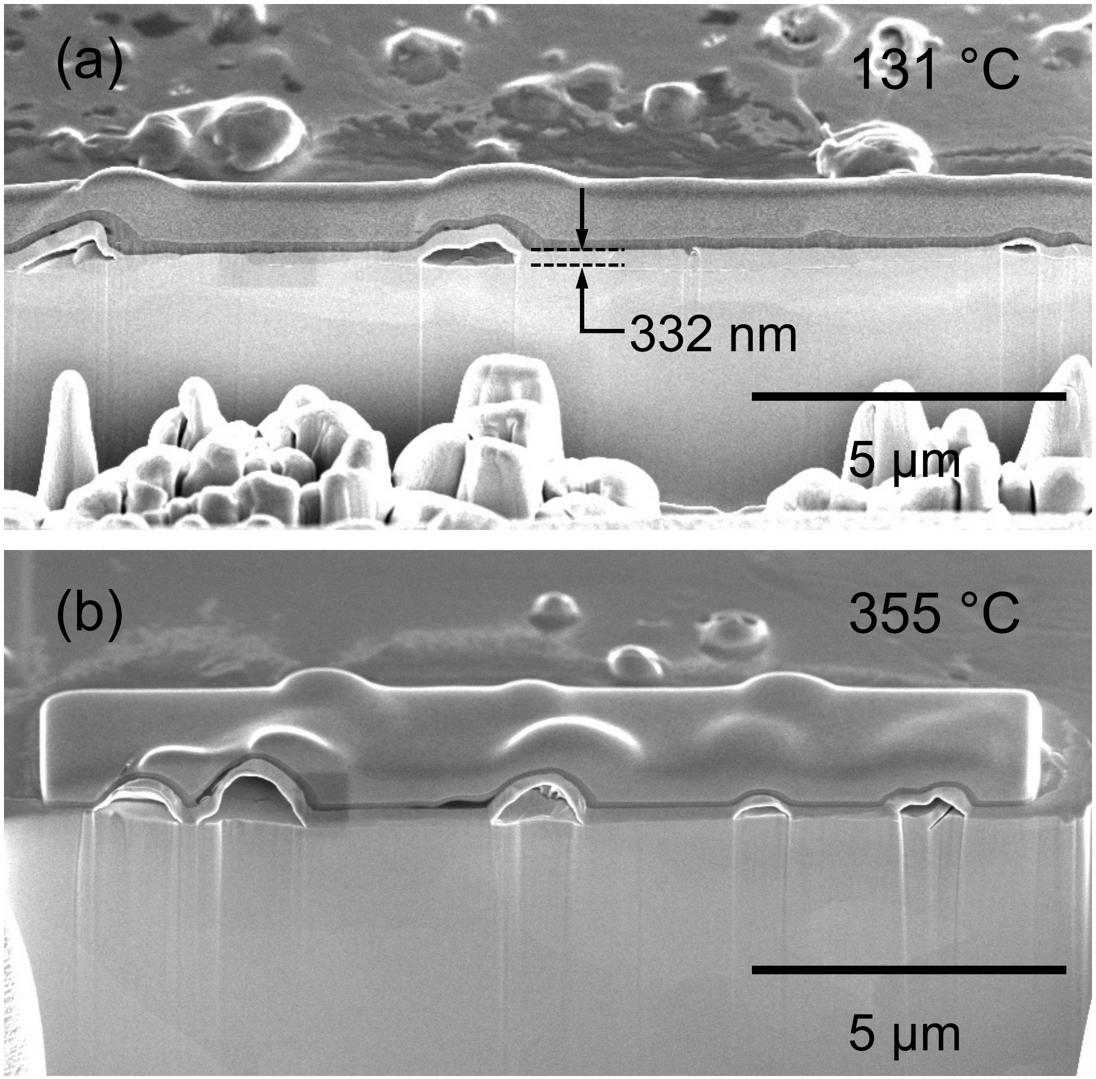

vacancy clustering



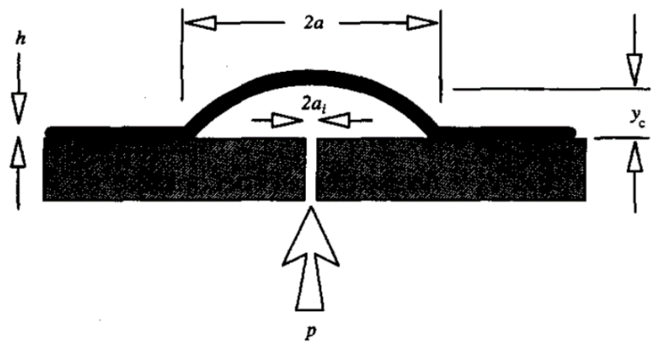

J. B. Condon & T. Schober, *J. Nucl. Mater.* **207** (1993) 1.

Mechanism that is active depends on exposure conditions as well as material microstructure

# Focused ion beam profiling reveals the nature of near surface precipitates



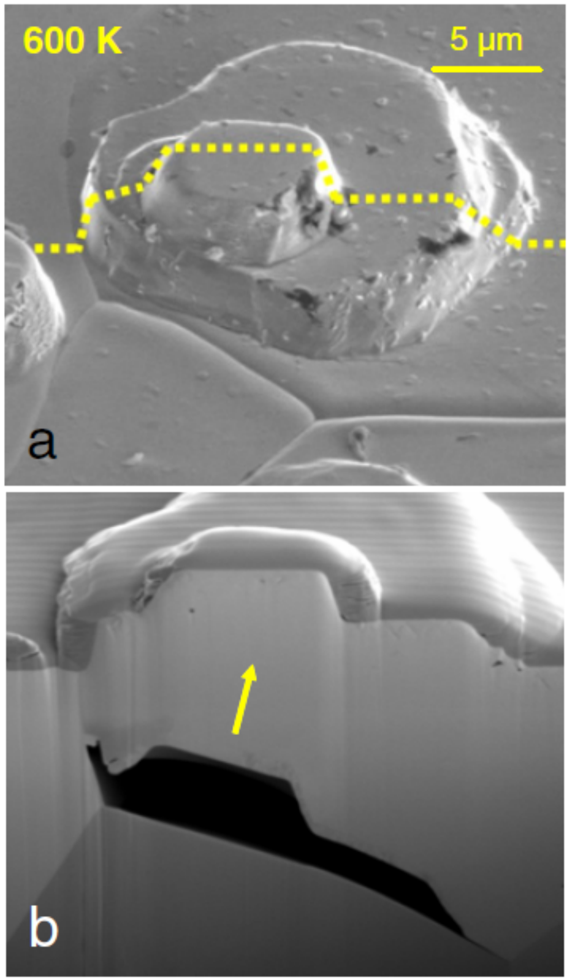

- Nucleation: platelet-shaped cracks
- Expansion due to internal gas pressure (> 1 GPa)




Proposed model:

$$p \geq \left( \frac{4T(Eh)^{1/3}}{5 C_1 C_2} \right)^{3/4} / r_b$$

# Dislocation loop punching enables precipitate growth far from the plasma exposed surface




S. Lindig, et al *Phys. Scr.* (2011)

**Stability condition**

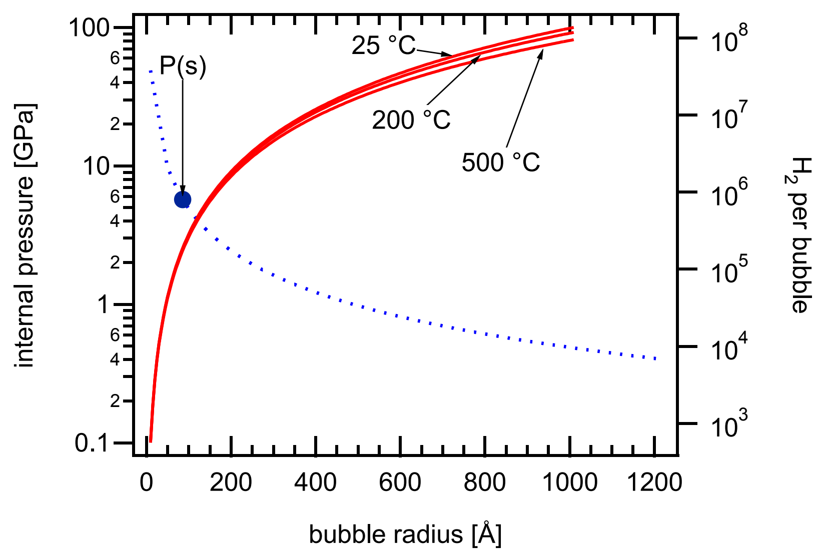
$p_{LP} \geq 2\gamma/r_b + \mu b/r_b$

$\gamma$ = surface energy

$r_b$ = bubble radius

$b$ = Burgers vector

$\mu$ = shear stress



# The internal pressure within $D_2$ - filled bubbles can exceed 1 GPa

**$H_2$ equation of state (EOS):**

P > 1 GPa expected within small bubbles.

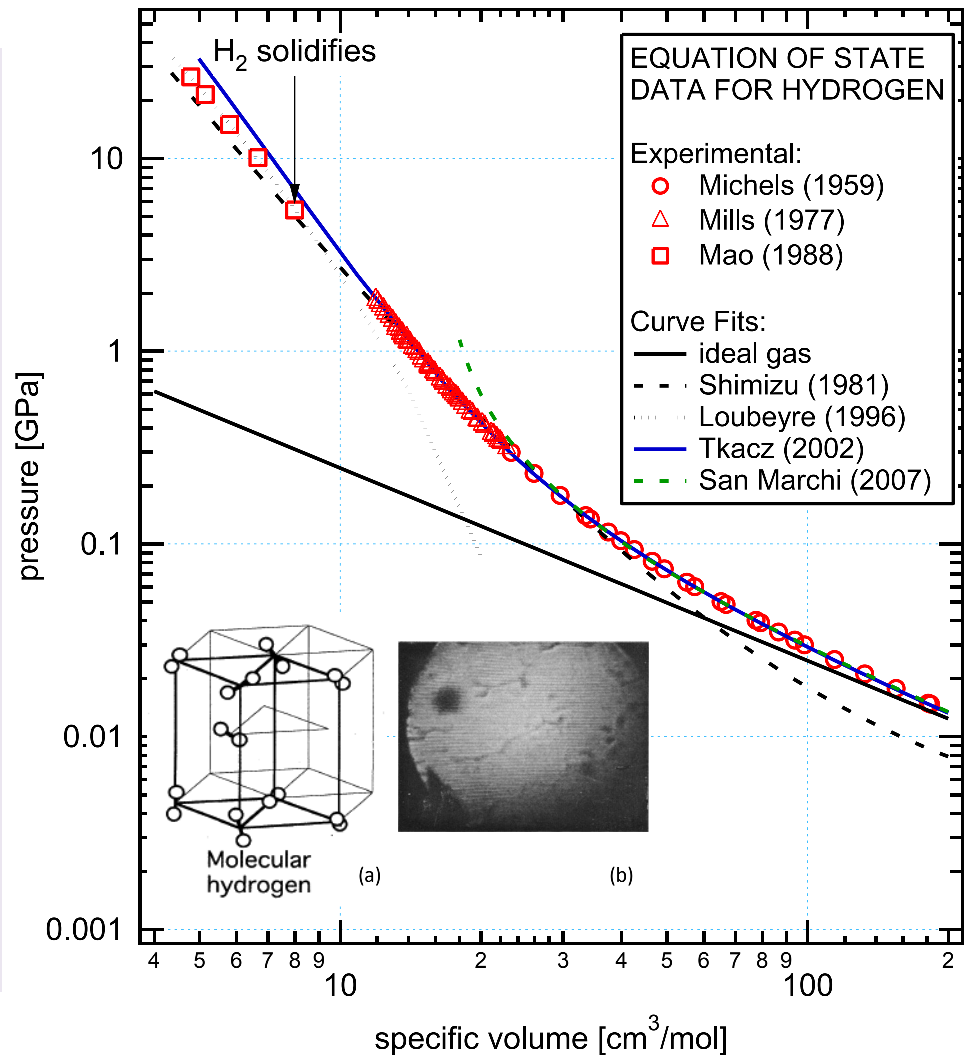
At 300 K, $H_2$ solidifies at p=5.7 GPa.

Tkacz's [J. Alloys & Compounds (2002)] EOS to provide the best fit:

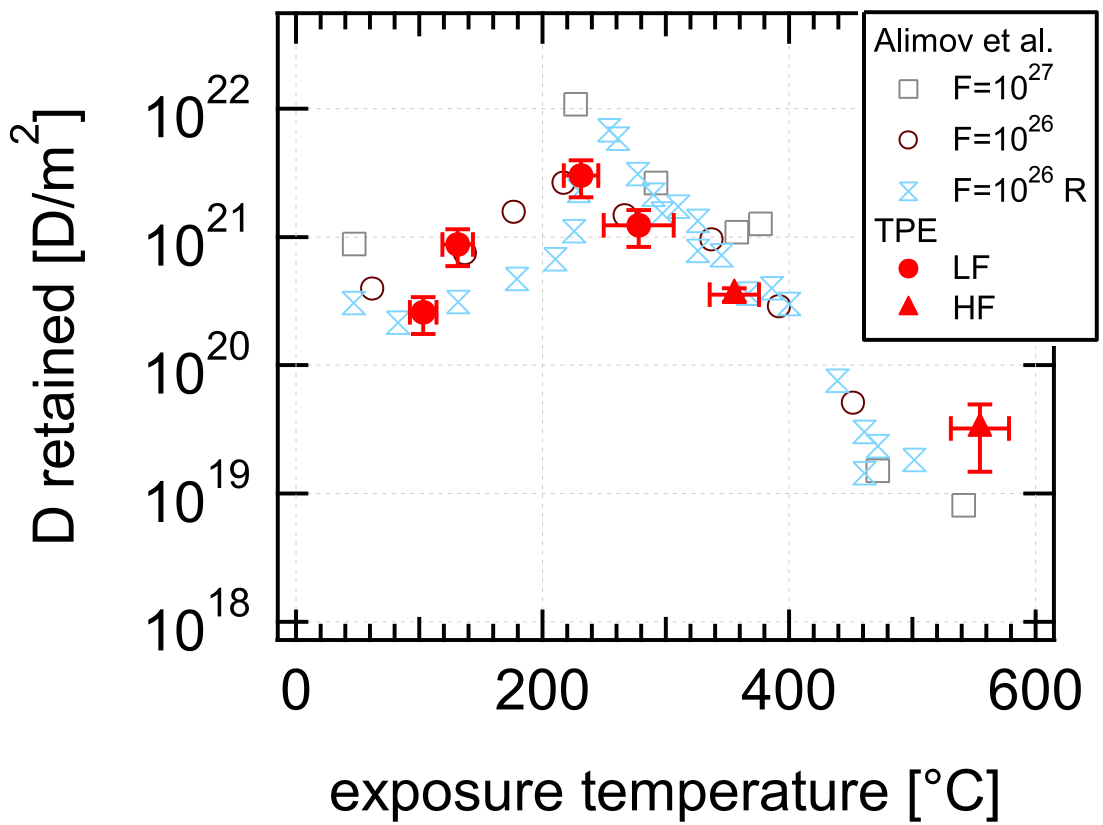
$$v = Ap^{-1/3} + Bp^{-2/3} + Cp^{-4/3} + (D + ET)p^{-1}$$

San Marchi's EOS better at low pressure:

$$v = \frac{RT}{p} + b$$



# Implications for tritium retention in ITER




**T < 200 °C**
Precipitation and trapping active, but slow diffusion

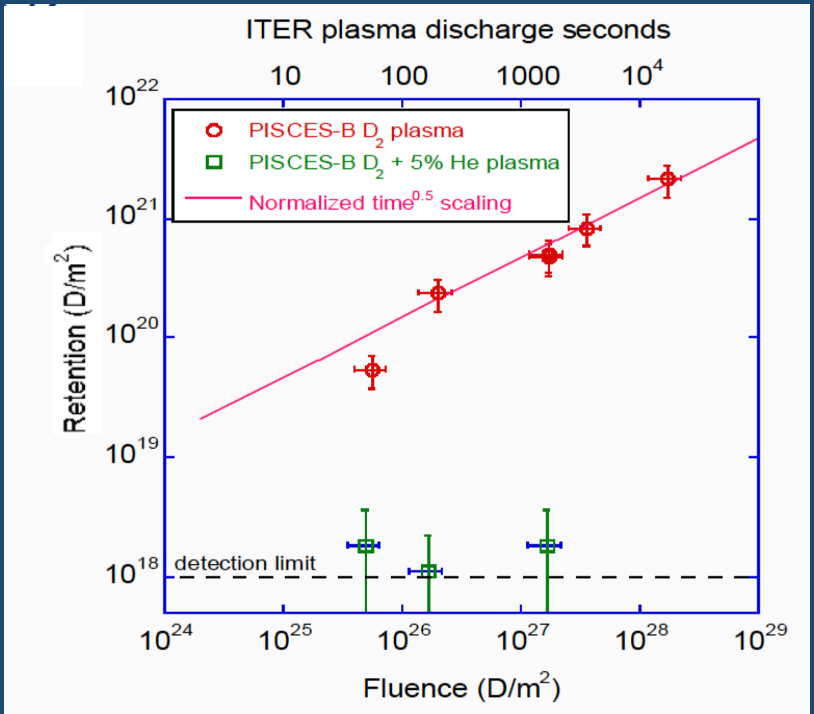
**200 °C ≤ T ≤ 300 °C**
Precipitation and trapping active, with fast diffusion

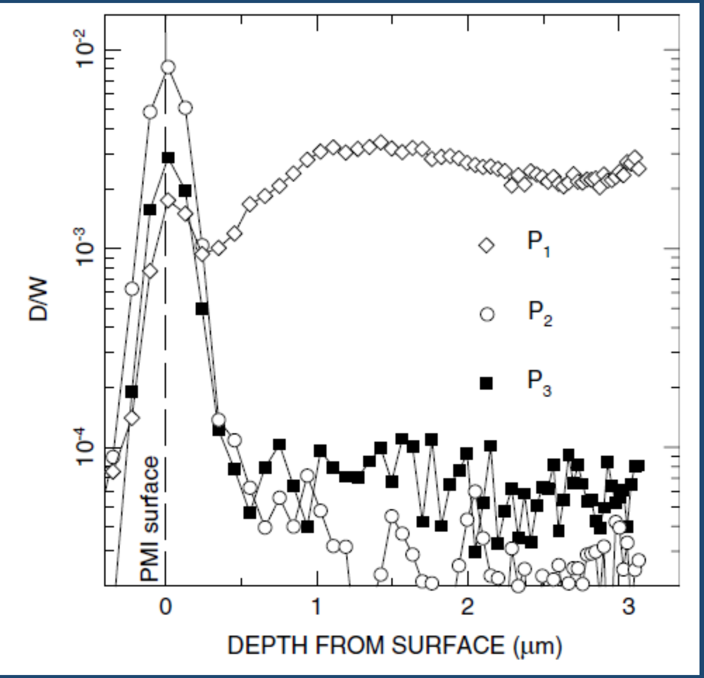
**T > 300 °C**
Small fraction of traps occupied, bubble expansion not favored.

# Helium effects: formation of near-surface nano-bubble structure leads to material degradation

Structure of first 100 nm – 1 μm of the surface governs:

- transport of T fuel through material
- sputtering → impurity transport into core plasma
- fuel recycling



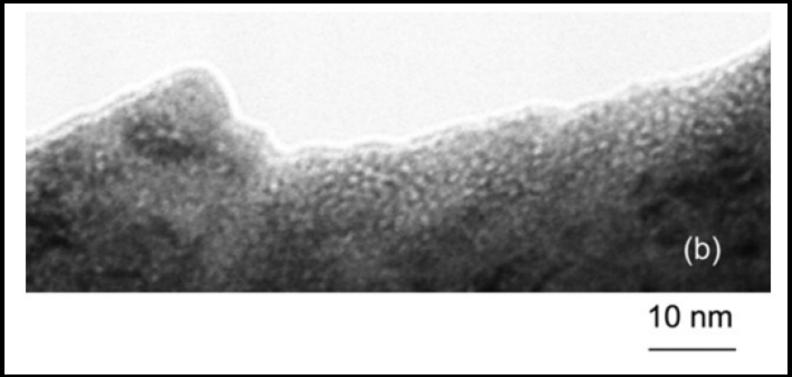




M. J. Baldwin, R. P. Doerner, W. R. Wampler, et al., *Nucl. Fusion* **51** (2011) 103021.

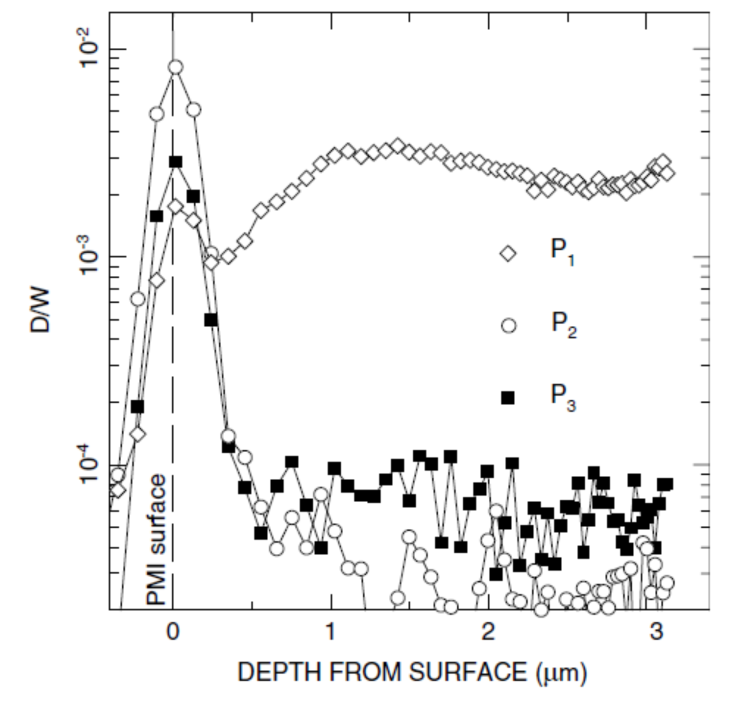
# Near-surface structure and composition integral to many aspects of fusion plasmas

Structure of first 100 nm – 1 µm of the surface governs:

- transport of T fuel through material
- sputtering → impurity transport into core plasma
- fuel recycling




Hypothesis: network of closely-spaced, nm-sized bubbles prevents deeper diffusion of implanted D into bulk.

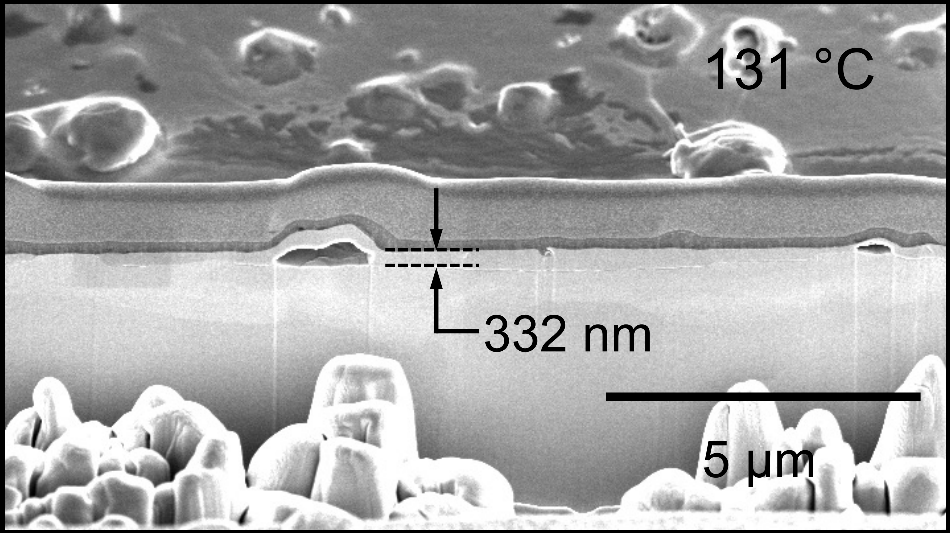



M. J. Baldwin, R. P. Doerner, W. R. Wampler, et al., *Nucl. Fusion* **51** (2011) 103021.

# Comparison: low-energy, high flux $D_2$ and He plasma-exposure

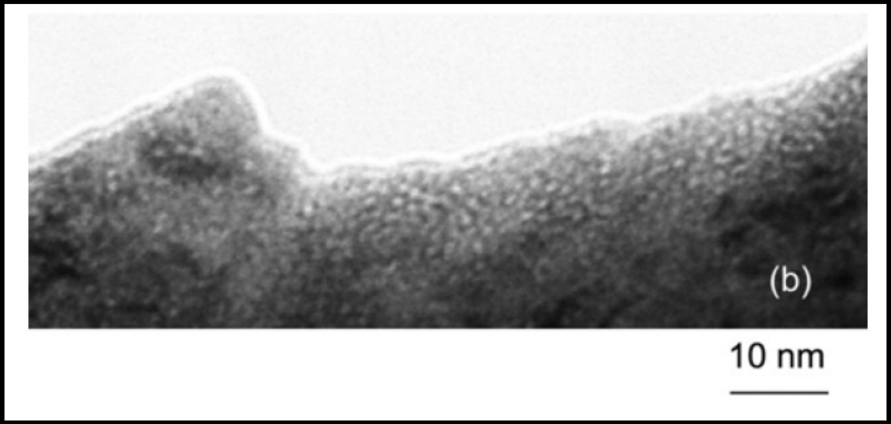
**Differences between $D_2$ and He precipitates in W:**
(a) He pair formation energetically favorable
(b) D migrates into the structure and nucleates blisters at pre-existing defects
(c) Depends strongly on existing microstructure

Blistering in D2 plasma




R. D. Kolasinski, M. Shimada, Y. Oya, D. A. Buchenauer, *J. Appl. Phys.* **118** (2015) 073301.

Near-surface bubble growth (He exposure)




M. J. Baldwin, R. P. Doerner, W. R. Wampler, et al., *Nucl. Fusion* **51** (2011) 103021.

# At high temperatures, high-flux He plasma exposure creates nm-sized filaments …

Advanced microscopies provide detailed insight into defects contained within different surface morphologies.

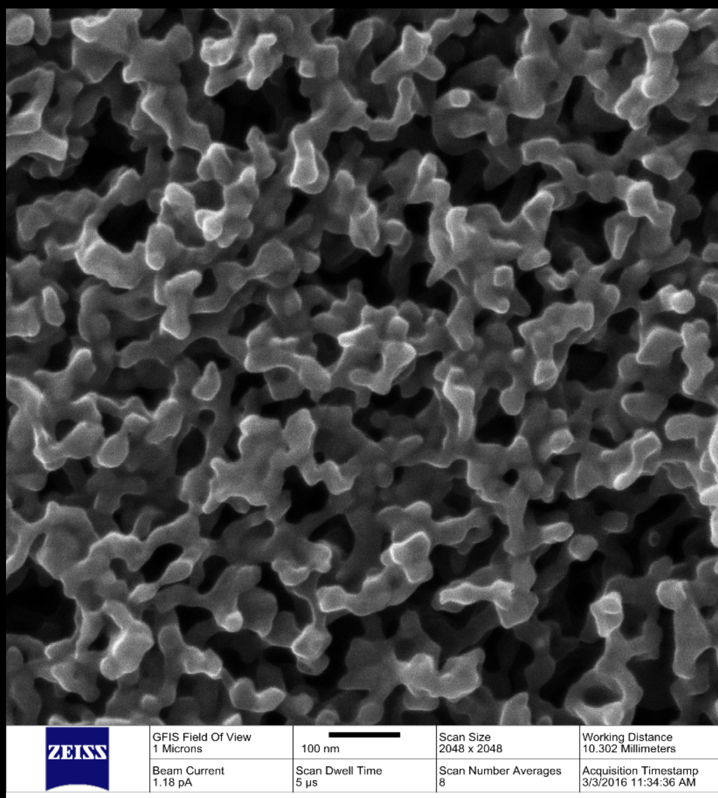
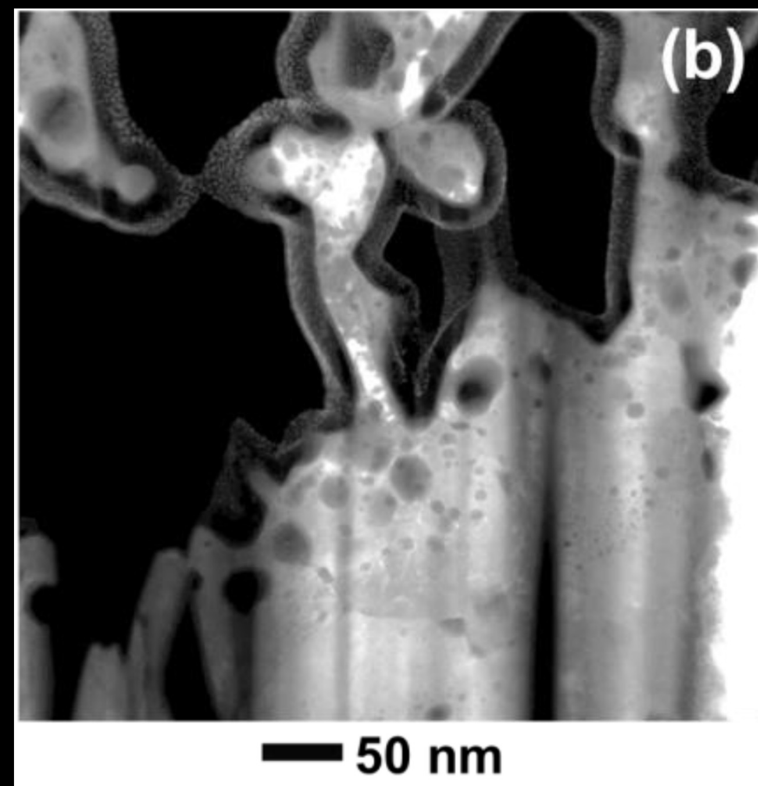
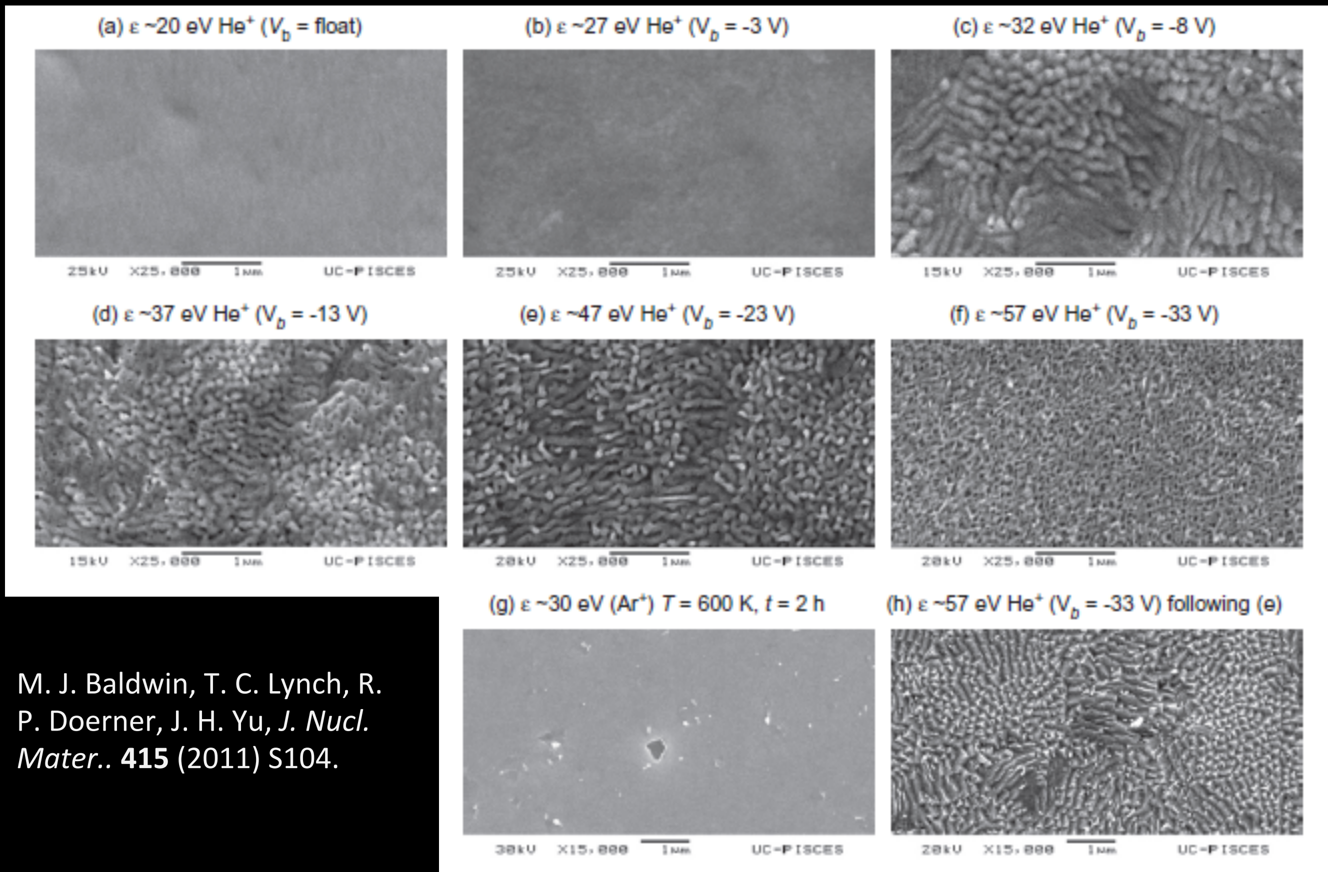



Image courtesy of F. Allen (U. C. Berkeley / LBNL)




Images from: C. M. Parish, R. P. Doerner, M. J. Baldwin, D. Donovan, K. G. Field, and Y. Katoh, *Microsc. Microanal.* **22** (2016) 1462.

# …whereas at lower temperatures / fluxes a dense layer of interconnected He bubbles forms.




M. J. Baldwin, T. C. Lynch, R. P. Doerner, J. H. Yu, *J. Nucl. Mater..* **415** (2011) S104.

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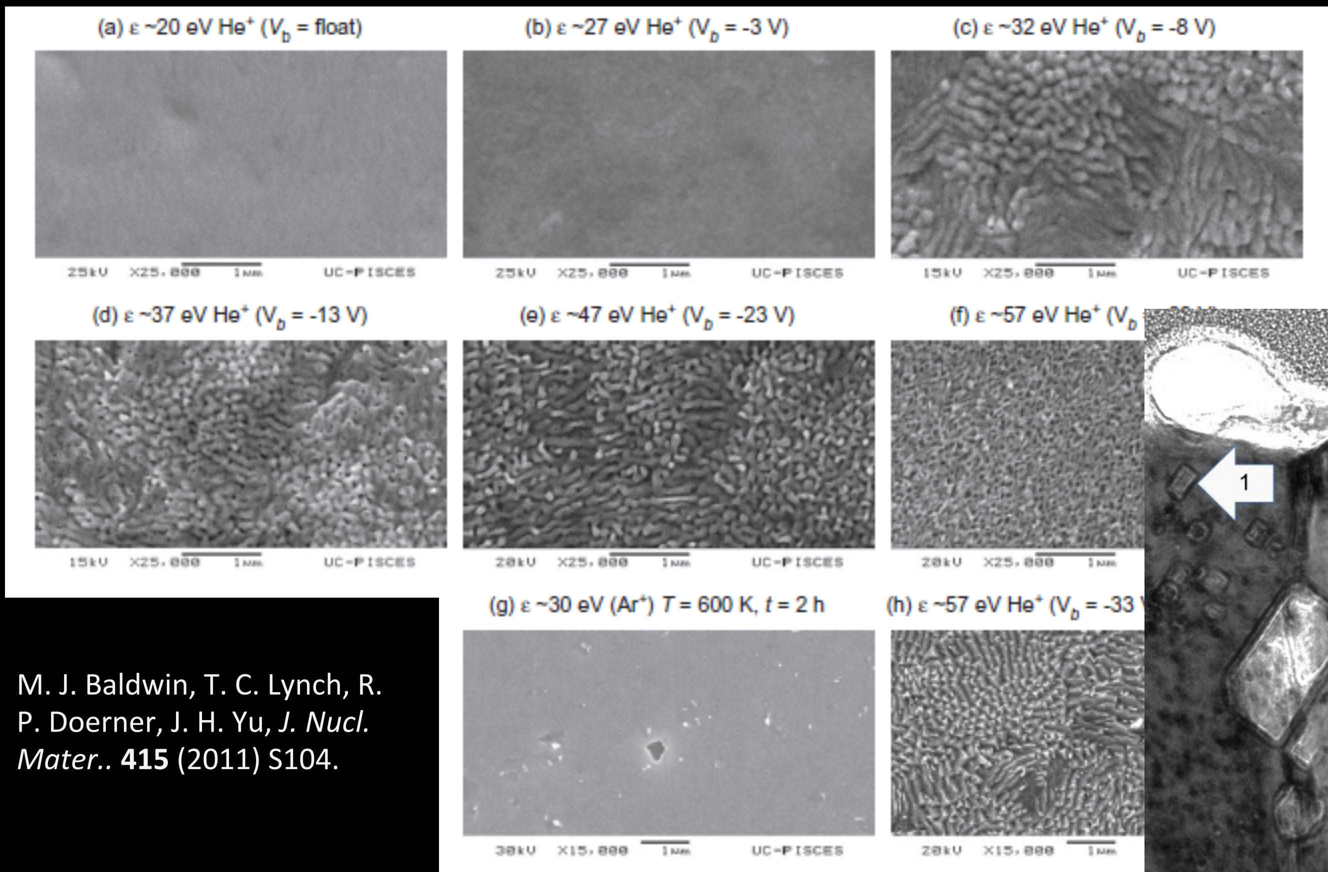
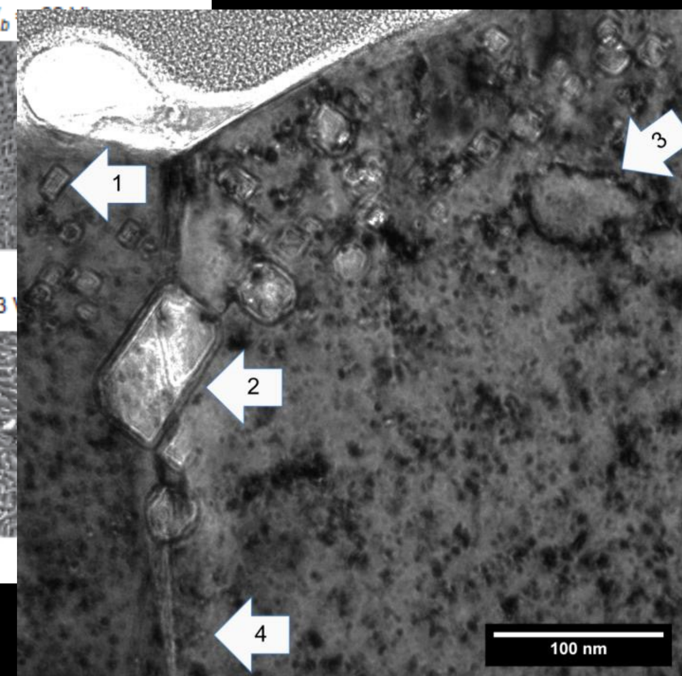



M. J. Baldwin, T. C. Lynch, R. P. Doerner, J. H. Yu, *J. Nucl. Mater.*. **415** (2011) S104.



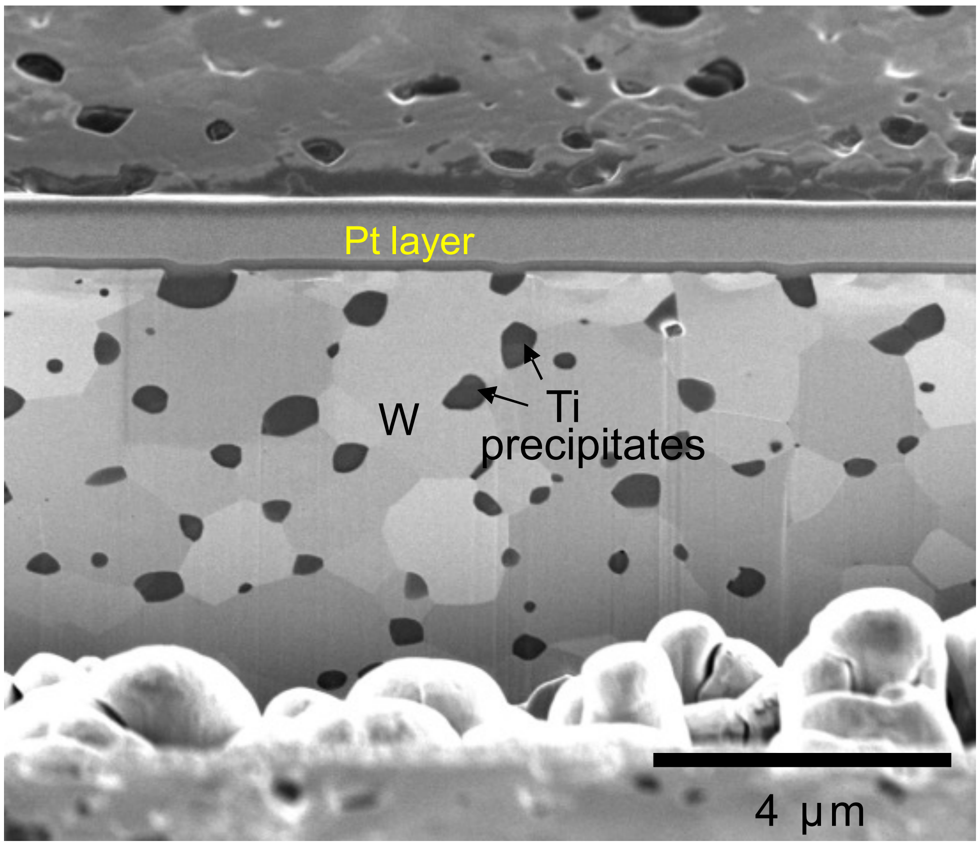

C. M. Parish, R. P. Doerner, M. J. Baldwin, D. Donovan, K. G. Field, and Y. Katoh, *Microsc. Microanal.* **22** (2016) 1462.

Advanced Concepts:
(a) W alloy development
(b) Liquid metal alloys
(c) In-situ diagnostic development

45

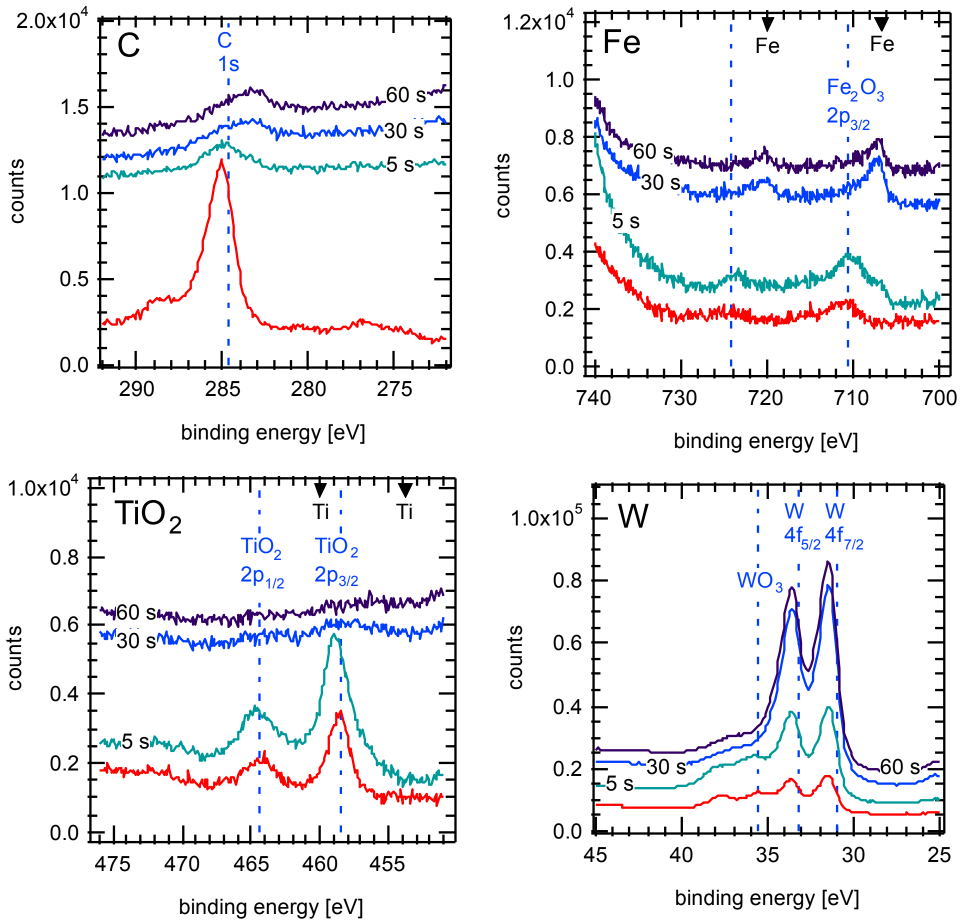
# Tungsten alloys may offer superior resistance to neutron damage and high heat loads

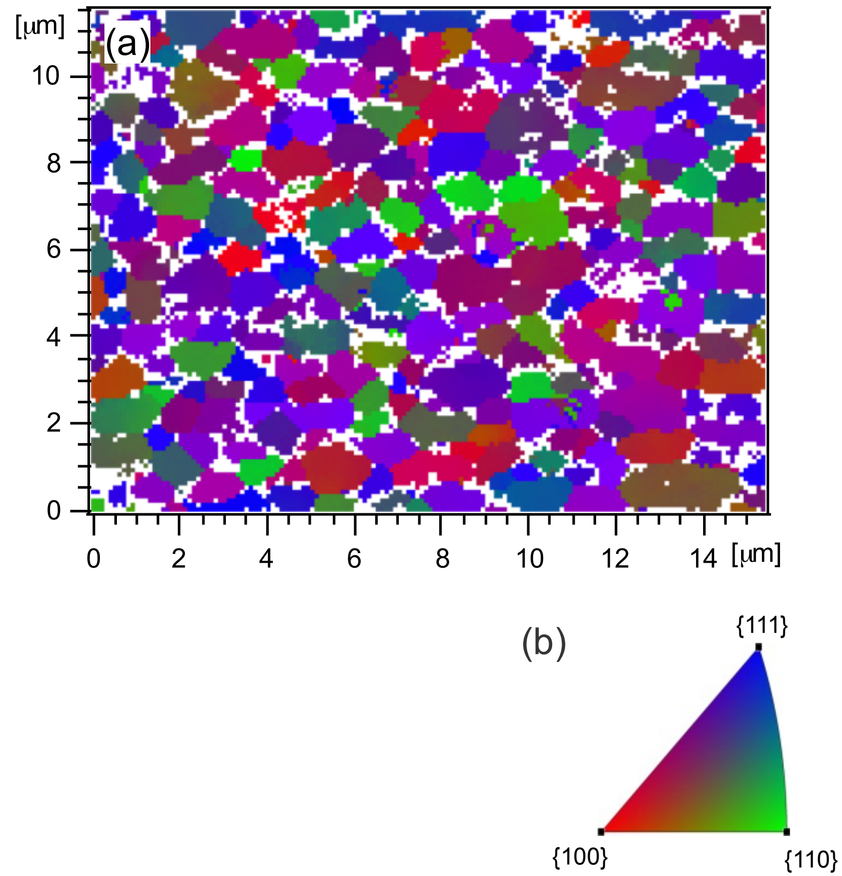
PMI Community Report emphasis on: *Novel materials and advanced manufacturing methods*




- W-Ti alloy developed at Univ. of Utah (Z. Fang)
- Microstructure offers possible resistance to neutron damage
- **Response to plasma unknown**
- Collaboration with UCSD for high-flux exposure

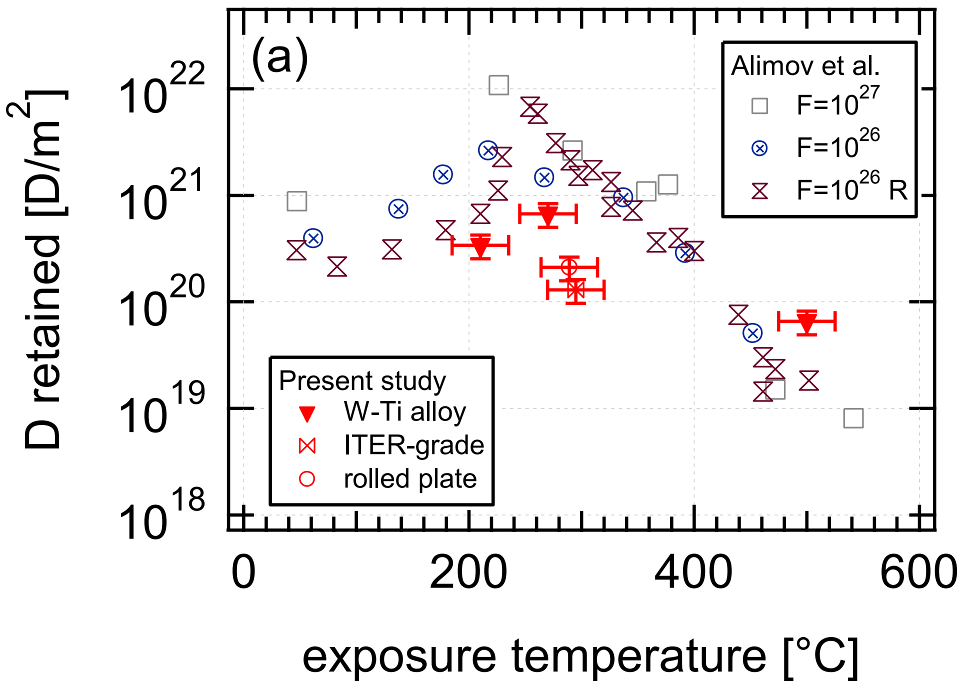
# Analysis of ultra-fine grained alloy produced by University of Utah



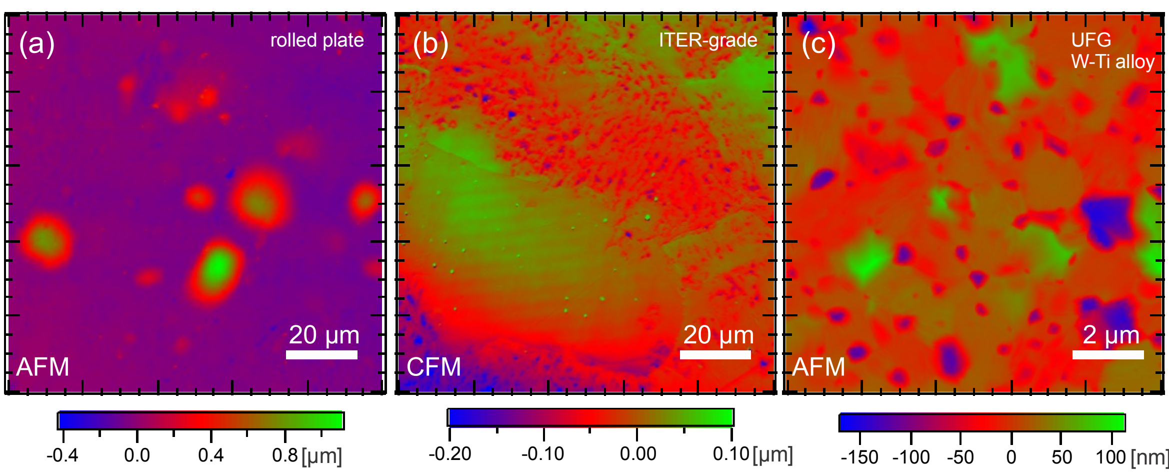




- XPS reveals dispersoids are $TiO_2$, unlikely to contribute to H diffusion
- EBSD data used to determine average grain size (960 nm), no preferred texture.

# W-Ti alloy exhibits improved resistance to surface modification, modestly increased retention



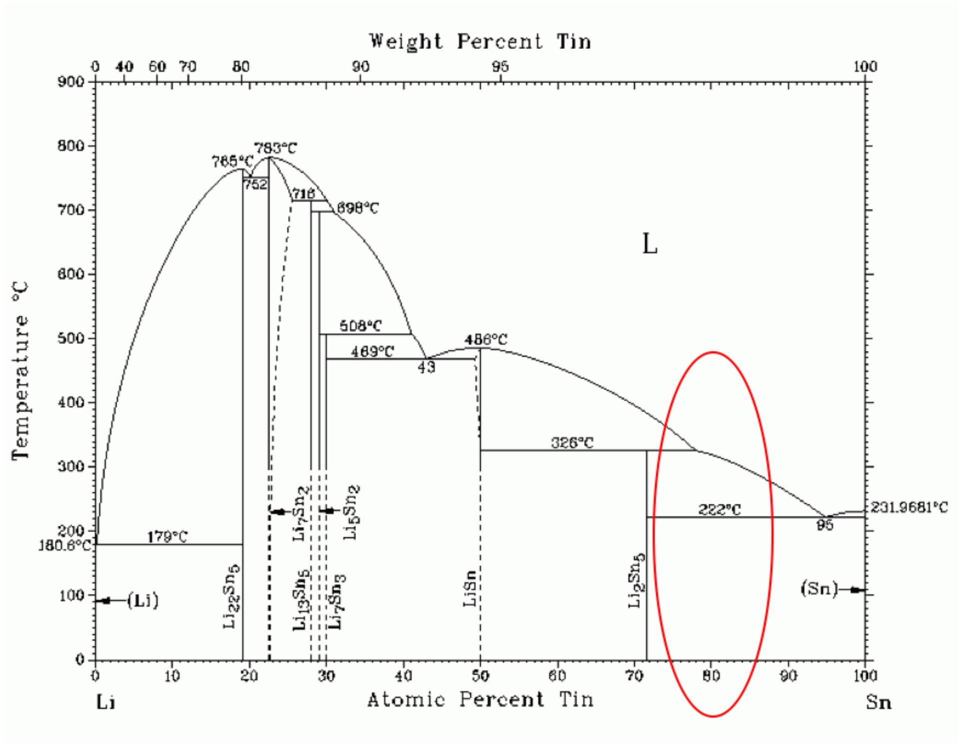

- Retention ~ 3 x higher than reference polycrystalline W
- Within typical range of variability for W grades
- Surface modification negligible




R. Kolasinski, D. A. Buchenauer, R. Doerner, et al., *Jnt. J. Ref. Met.* (2016).

# Liquid metal alloys offer possibility to avoid many problems associated with solid surfaces

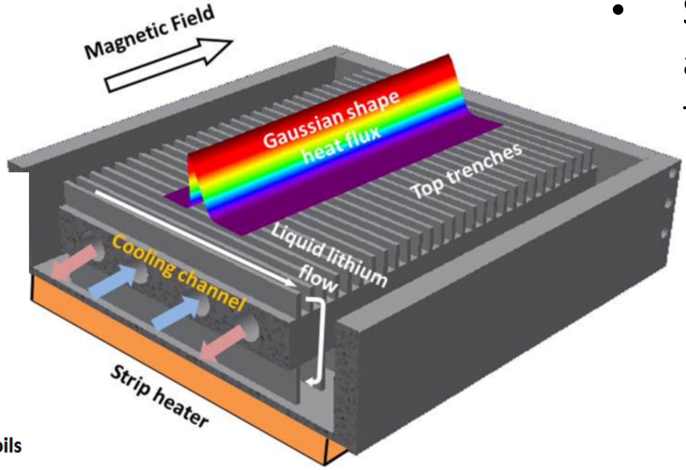
- Low melting Sn-Li eutectic has been proposed as an alternative to pure Li as a plasma facing surface
- Sn-Li 80:20 mixture projected to be able to handle the projected heat loads
- Due to lower surface energy, Li segregates to the surface during melting, and would act as a low-recycling wall, with improved retention characteristics.
- Sn-Li has fewer chemical reactivity issues and higher material compatibility.
- Currently under investigation at University of Illinois / Princeton



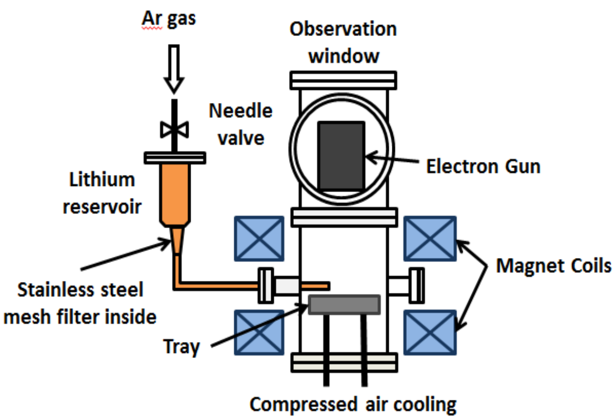
# Liquid metal infused trenches (LiMIT)

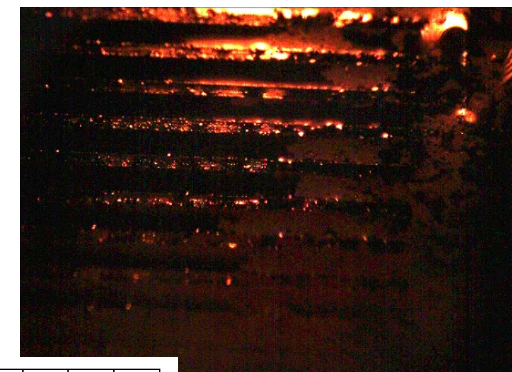
## LiMIT is a versatile system for testing liquid metal flows for PFC applications

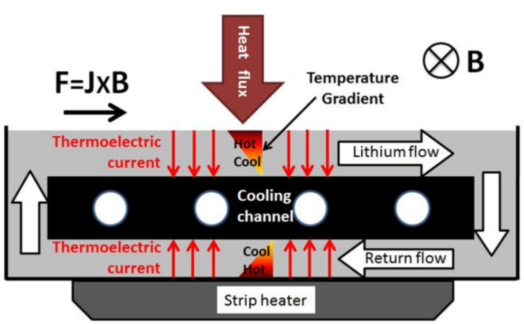
- Horizontal Flow
- Utilizes TEMHD drive for propulsion of liquid lithium through a series of trenches

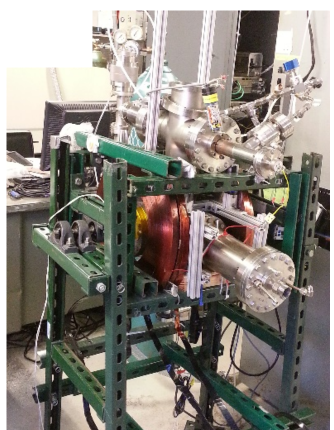


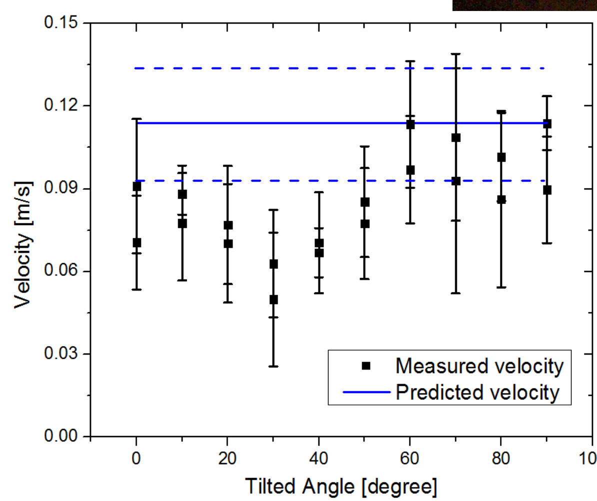

- Vertical Flow (and arbitrary angle)
- Sustained flow demonstrated at arbitrary angle from horizontal ($0^o$ to $180^o$)



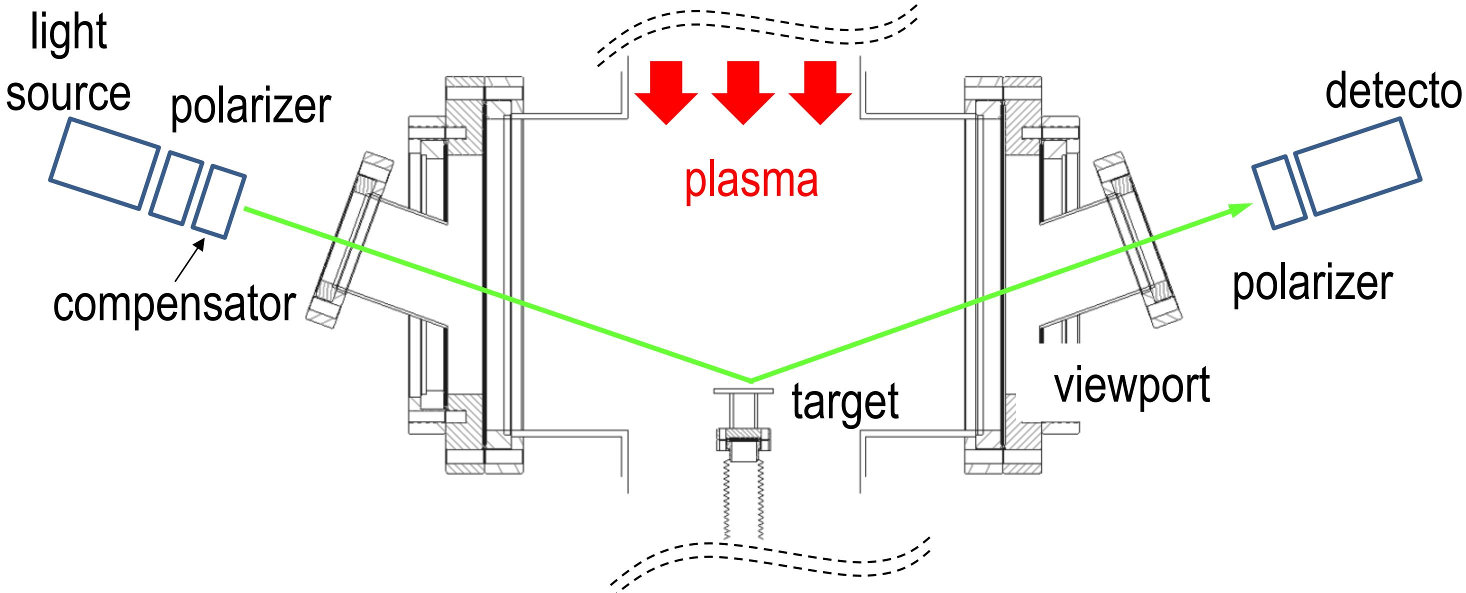





PI: David Ruzic (University of Illinois)

# In-situ optical diagnostics: spectroscopic ellipsometry




- Measures polarization angles, ψ and Δ which characterize the polarization state change of light reflected from the sample:

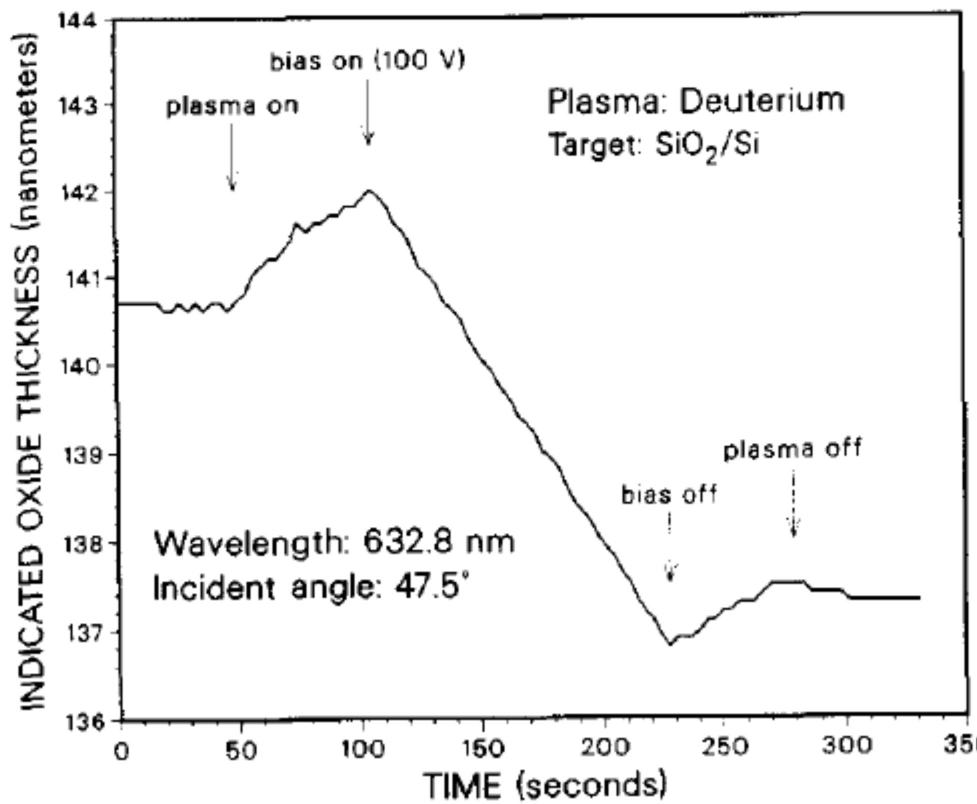
$\rho = r_p / r_s = \tan(\psi)\exp(i\Delta)$

- Note: ρ = reflectivity, $r_p$, $r_s$ are reflection coefficients of p and s waves.
- Used frequently to determine optical thickness of films

# Previous demonstration on PISCES-B

Prior work by Bastasz tested feasibility:

- Used single-wavelength ellipsometer to measure $SiO_2$ erosion from Si substrate.
- Achieved 1 nm depth resolution, with 1 Hz sampling frequency.
- No adventitious effects of the plasma on ellipsometer signal observed.
- Alignment of the optical hardware posed the largest practical issue



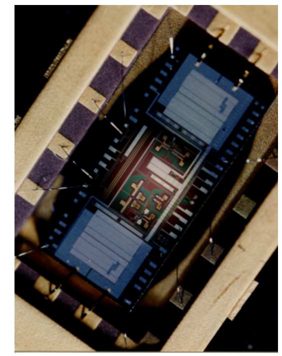

R. Bastasz, Y. Hirooka, and M. Khandagle, *J. Nucl. Mater.* **220** (1995) 352.

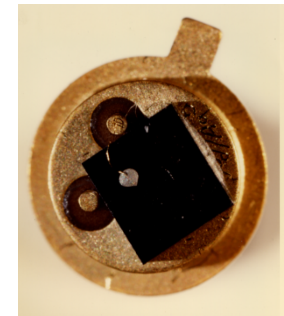
# In-situ diagnostics: Hydrogen micro-sensor development

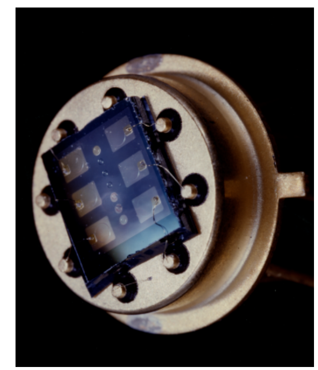
**C-X measurements on existing tokamaks are limited to high energies and usually one location**

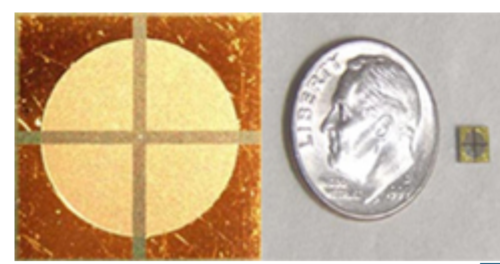
**Pd-MOS detector development**

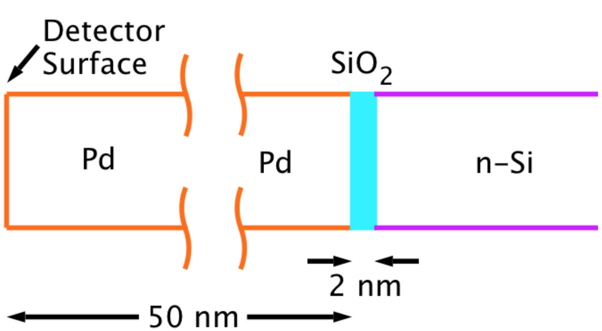
- Small size, low voltage, high sensitivity detectors provide dosemetric measurements
- Energy resolution can be obtained through Au overlayers
- Partner with Mesafab at SNL-NM to develop radiation resistant detectors
- Characterize using m&E filtered ion beam at SNL-CA

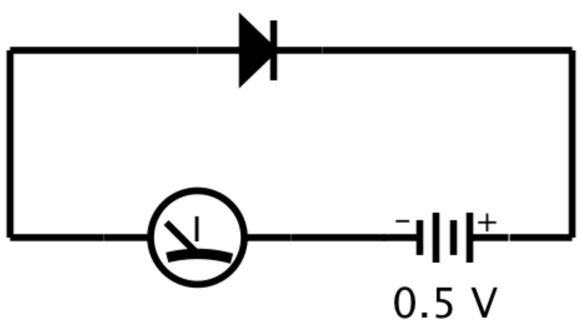










# Concluding Remarks

**Plasma material interactions likely to be a key focus for fusion research going forward:**

- *Key issues*
  - Tritium retention / migration
  - Degradation of near-surface structure due to shallowly implanted D and He
  - Sputtering / redeposition
  - Neutron damage
- *Future directions*
  - Development of advanced PFC concepts (tungsten alloys or liquid metal systems)
  - New in-situ diagnostics will bring further insight into physics underlying PMI

# Acknowledgements

I would like to express my appreciation to:

- My colleagues at Sandia/CA:
  - Dean Buchenauer, David Donovan, Richard Nygren, Josh Whaley, Jon Watkins, Thomas Felter
- Our collaborators:
  - Brian Wirth (Univ. of Tenn.), David Donovan (Univ. of Tenn.), Masa Shimada (INL), Brad Merrill (INL), Matt Baldwin (UCSD), Russ Doerner (UCSD), Dmitry Rudakov (UCSD), Clement Wong (GA), Bruce Koel (Princeton), David Ruzic (Univ. of Illinois)

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