Plasma Surface Interactions (PSI) Science Center

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Presented at the
Plasma Facing Components 2011 Meeting
Oak Ridge National Laboratory
10 August 2011

3 MIT Alcator C-Mod

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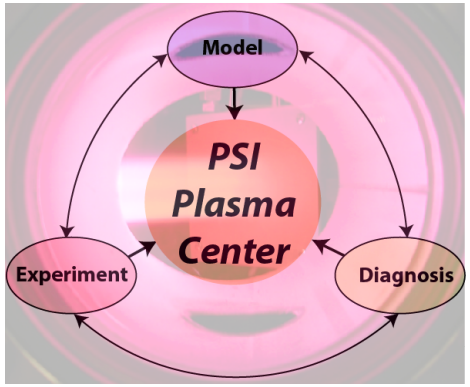

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6 DIII-D NATIONAL FUSION FACILITY SAN DIEGO

3 UCSD University of California San Diego

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OAK RIDGE National Laboratory

Presentation Overview

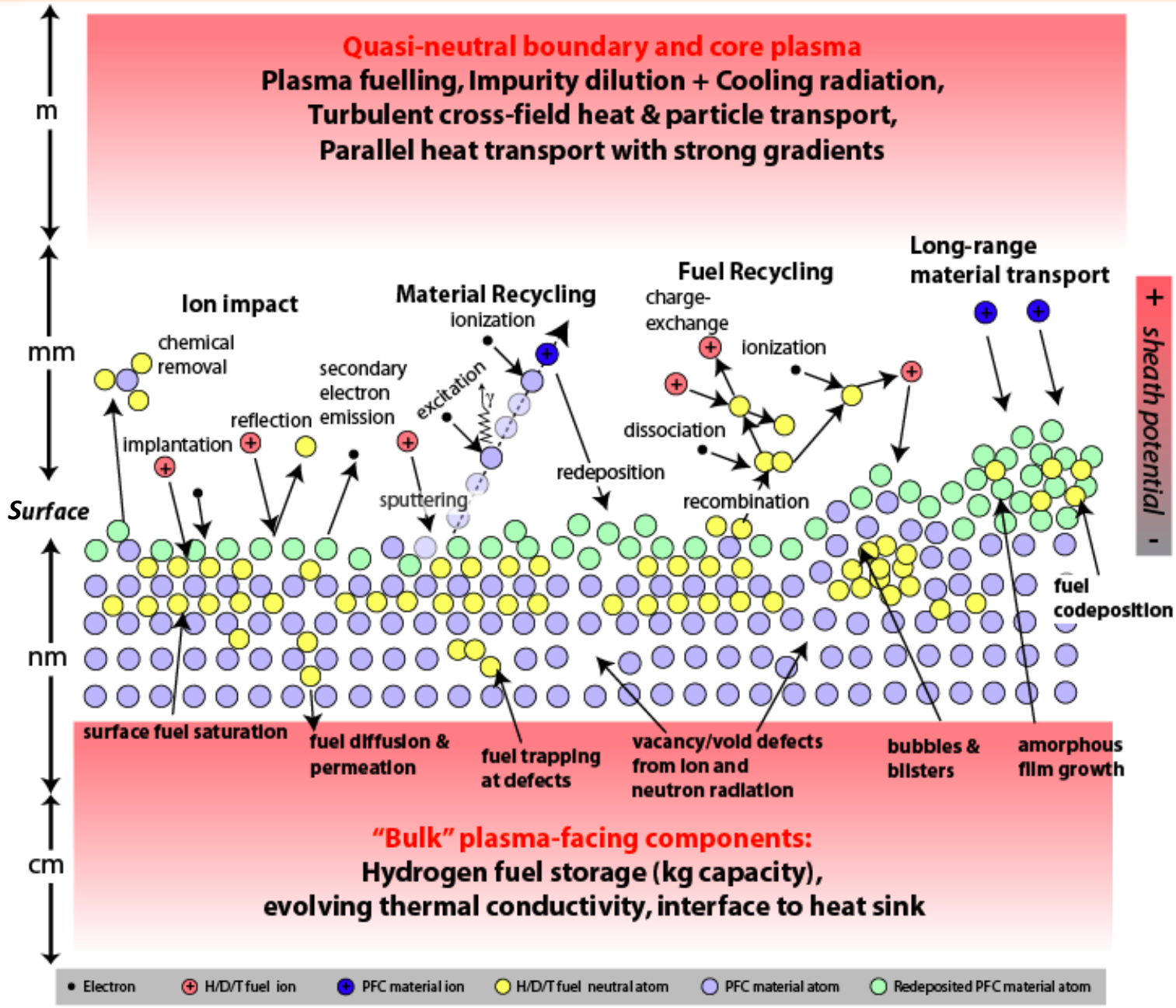
- **Challenges of plasma facing components & structural materials in the (magnetic) fusion environment**

- **Introduction to goals, organization, research approach and capabilities of the PSI Science Center**
  - Still a work in progress, but beginning to integrate wide range of exposure, diagnostic and modeling techniques

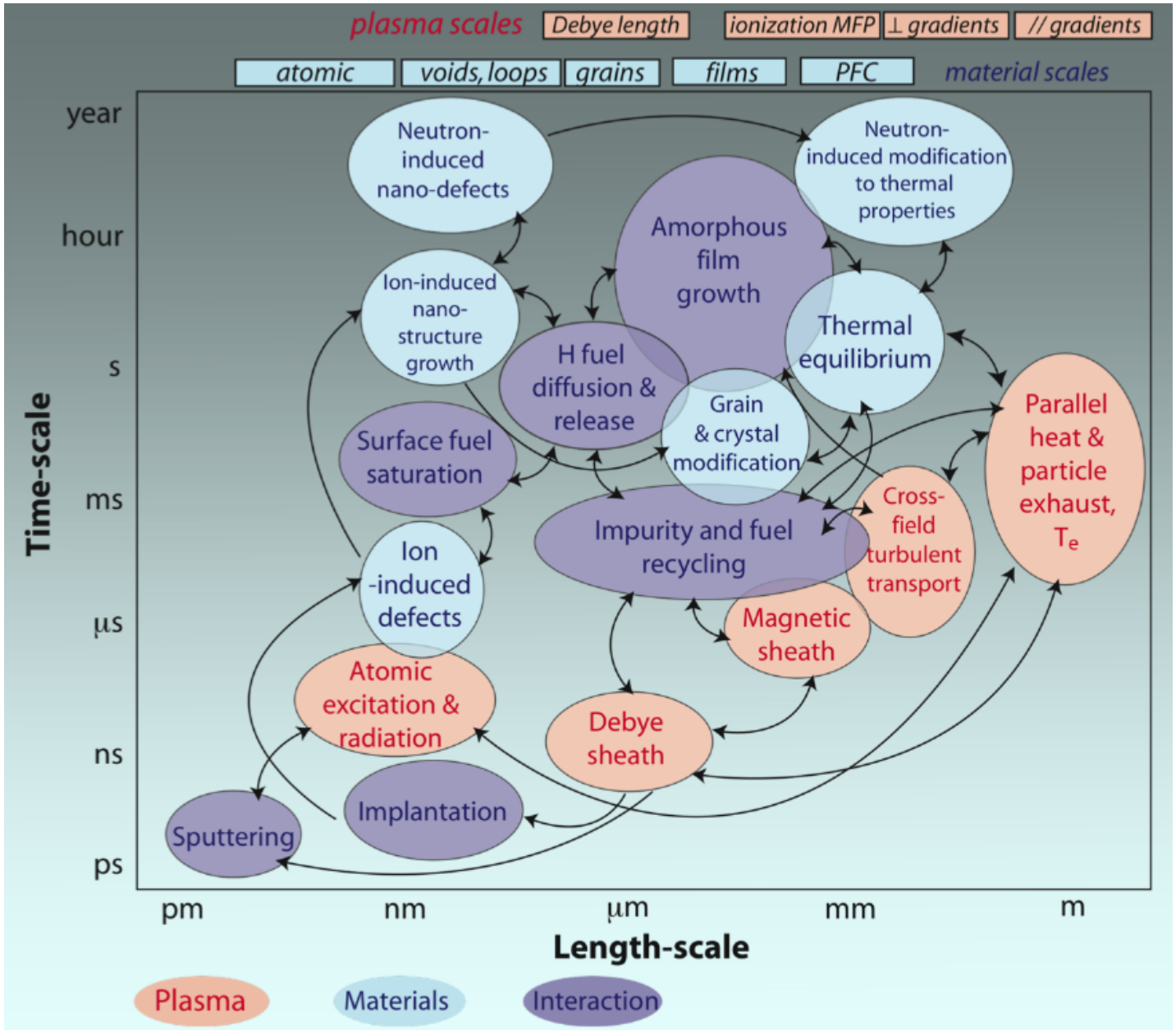
- **W fuzz formation mechanisms:**
  - Experimental capability development & initial characterization
  - Molecular dynamics modeling to investigate sub-surface He bubble stability
  - Model of fuzz formation

- **Summary and future work**

Multiscale, synergistic plasma surface interface



*Multiscale challenge of PSI Science**



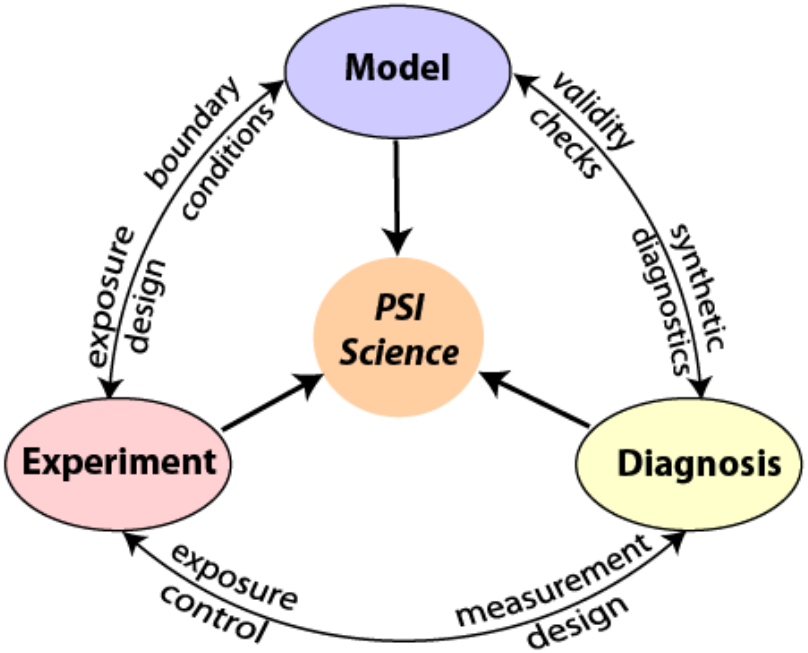
* Wirth, Nordlund, Whyte, and Xu, *Materials Research Society Bulletin* **36** (2011) 216-222

PSI Science Center Goals

- **Advance basic science understanding of plasma-surface interactions**

- **Strong external impact by bridging the gap between "laboratory" PSI studies and "real-world" applications**
  - **Magnetic fusion**
  - **Plasma thrusters**
  - **Plasma processing**

- **Develop and train the required new generation of multidisciplinary PSI scientists.**



PSI Science Center Organization

- **Consistent with our "tripod" research paradigm, Center leadership and funding (1400 k$) is distributed roughly equally among**
  - **University of Tennessee -- Materials modeling : Brian Wirth (300 k$)**
  - **UCSD -- PISCES / WallPSI model / DIII-D : Russ Doerner (525 k$)**
  - **MIT -- DIONISOS / Accelerator lab / C-Mod : Dennis Whyte (450 k$)**

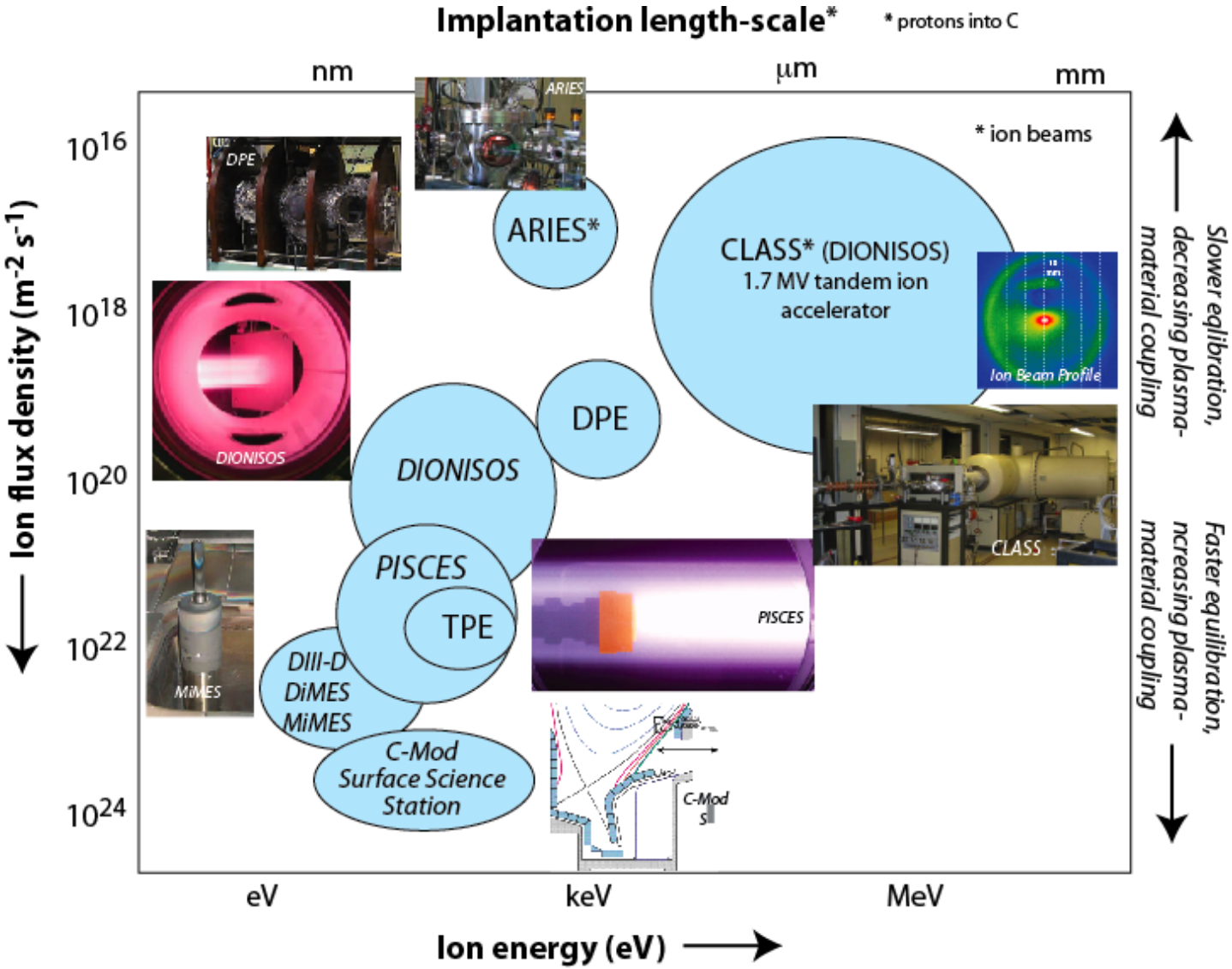
- **Collaborative outreach and participation of major tokamaks and national labs**
  - **General Atomics, LLNL, Alcator C-Mod, AdAstra Rockets, JPL**
  - **Support for PSI lab facilities of Sandia / CA: Dean Buchenauer (125 k$)**

- **Over 90% of funding to universities.**

- **Supports 12 young scientists / students**
  - **Strongly leverages coordination of existing hardware.**

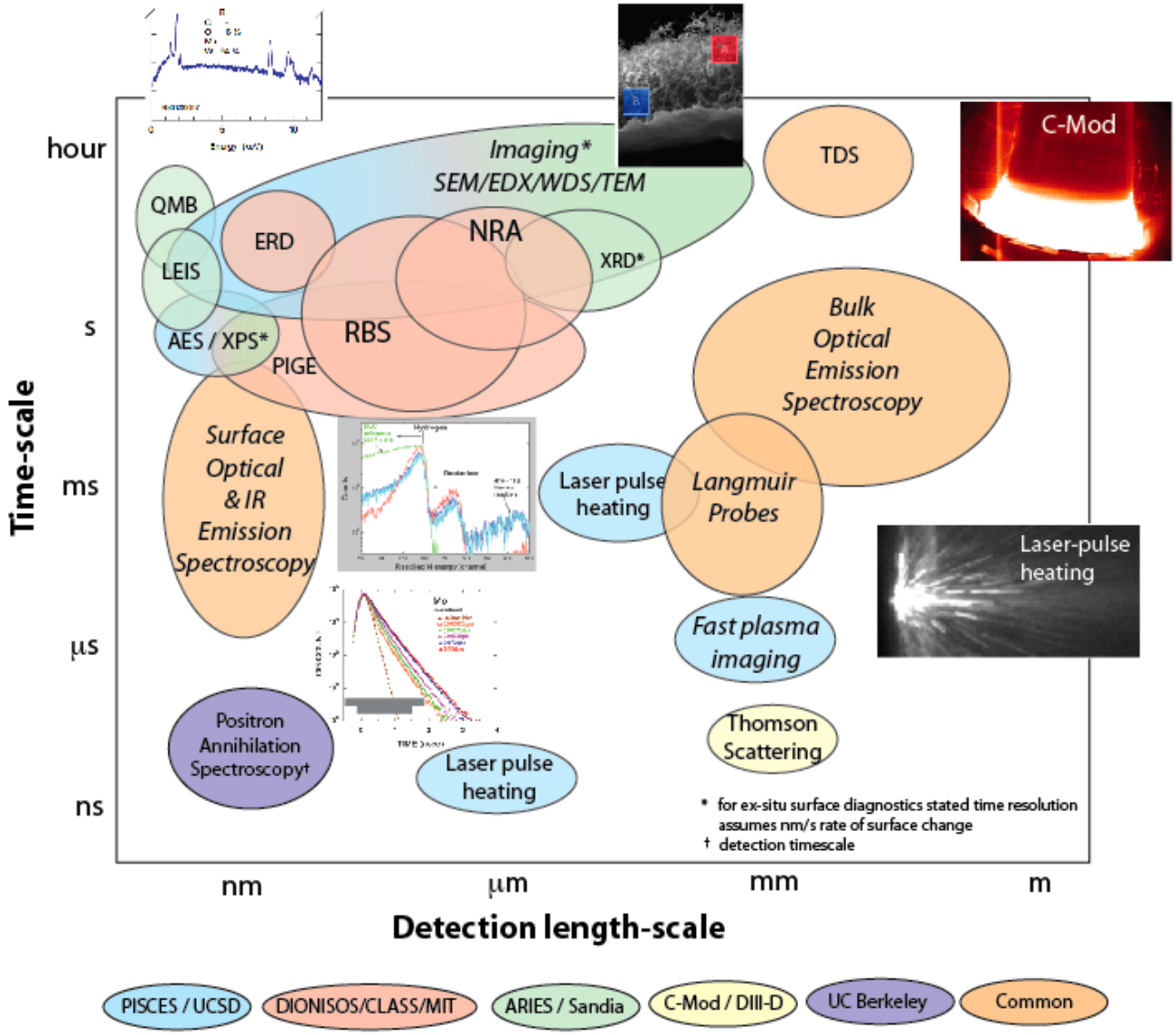
PSI Exposure capabilities

- *An integrated Center, including tokamaks, covers range not possible in single facility*



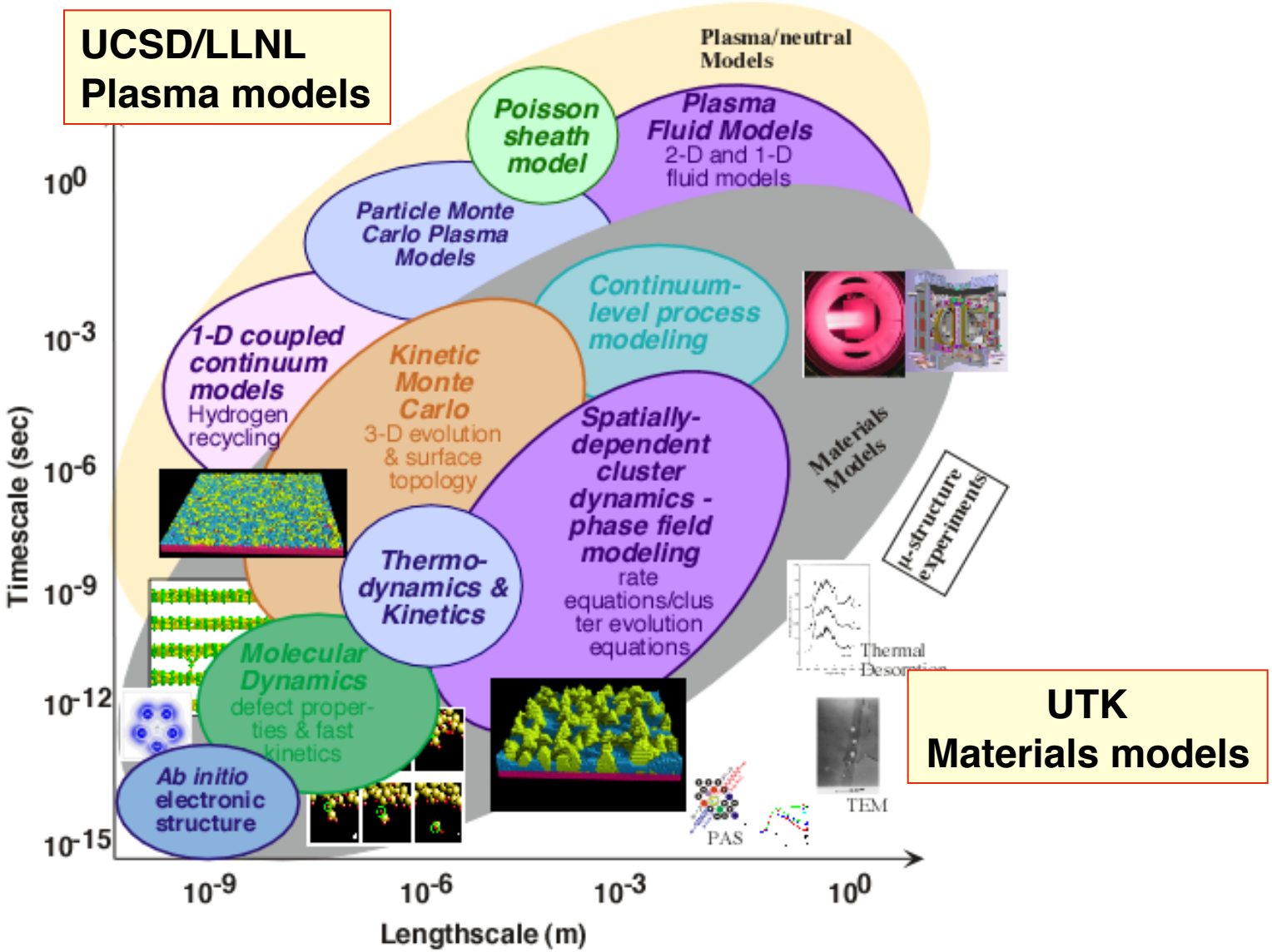
PSI Diagnostic capabilities

Integrated tools for surface/plasma measurements, including unique DIONISOS in-situ ion beam analysis



PSI Modeling capabilities

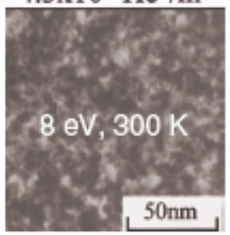
Integrate validated multiscale models of materials, plasma-surface interface and plasma



Surface dynamics under combined thermal/particle fluxes

T < 700 K

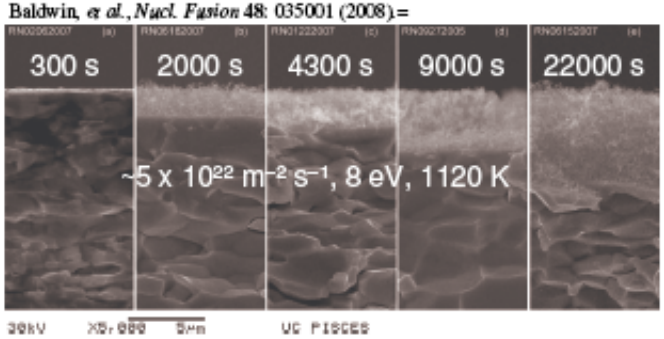
4.3x10^{19}He^{+}/m^{2}



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

non-specific damage

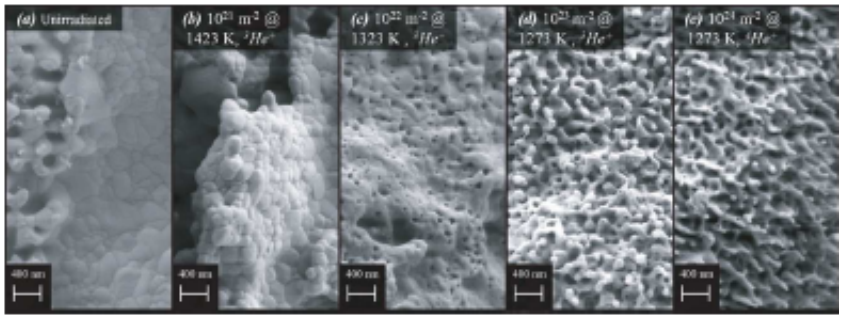
Baldwin, *et al.*, *Nucl. Fusion* 48: 035001 (2008).



900 K < T < 1900 K

fuzz / coral

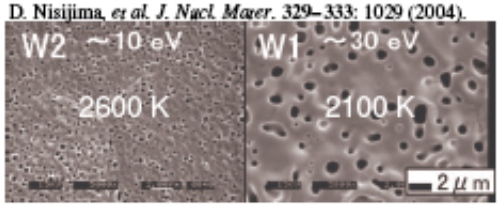
S. J. Zenobia and G. L. Kulcinski. *Phys. Scr.* T138: 014049 (2009).

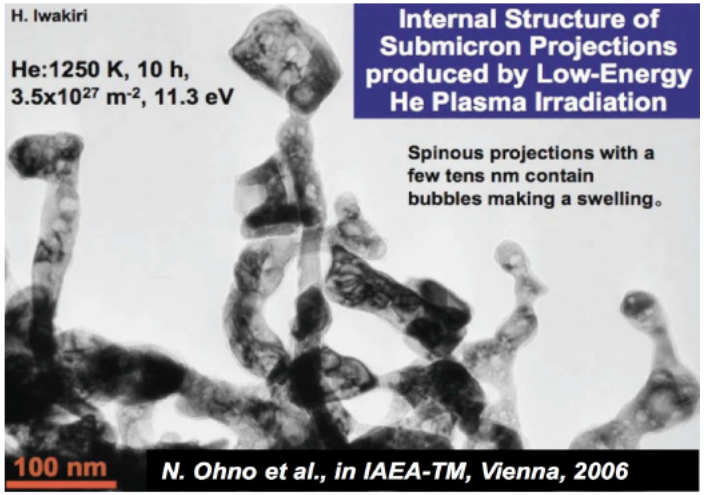


T > 2000 K

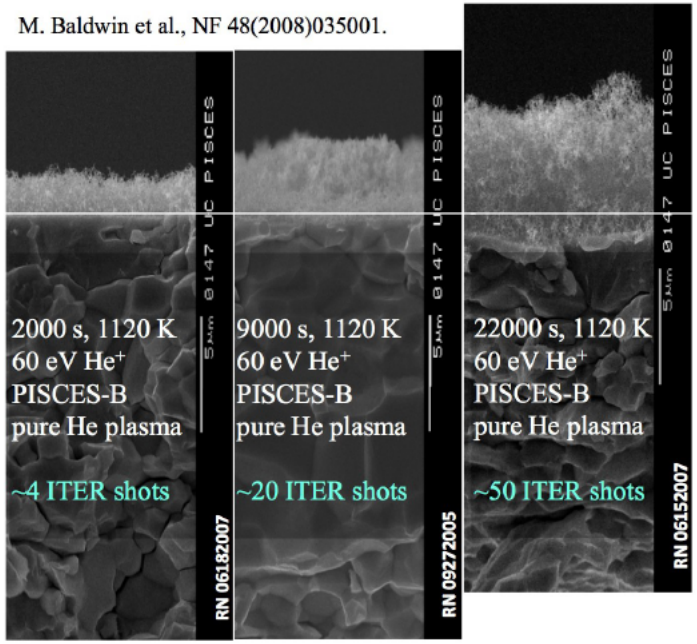
holes

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





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



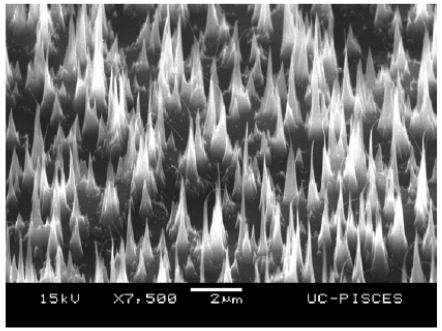
Plasma composition effects morphology & yield

pure D_2 (tmsBe17)

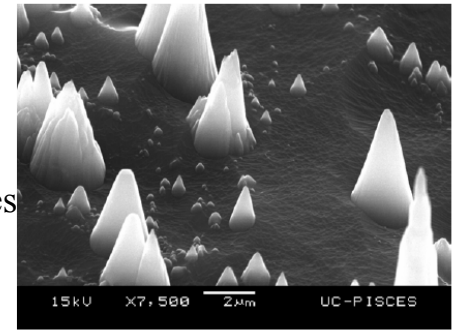
Y= 0.45% per ion

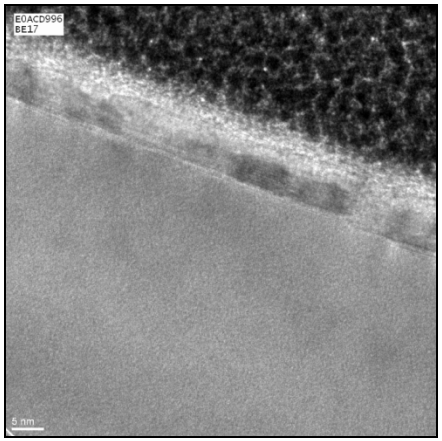
20% Ar in D_2 (tmsBe18)

Y= 1.4% per ion

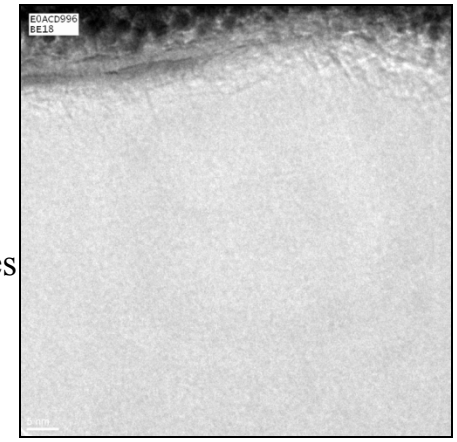


SEM images



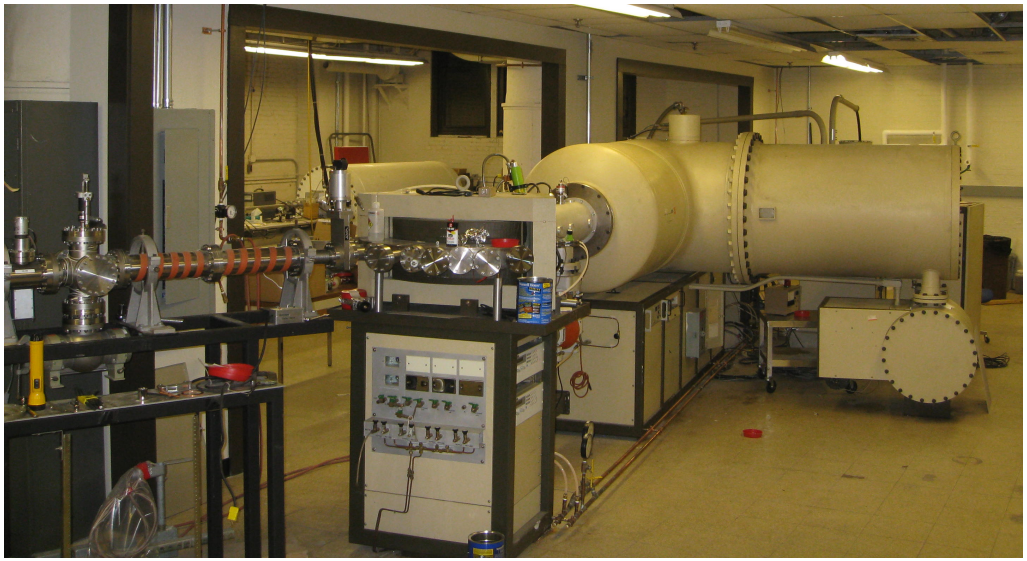


TEM images

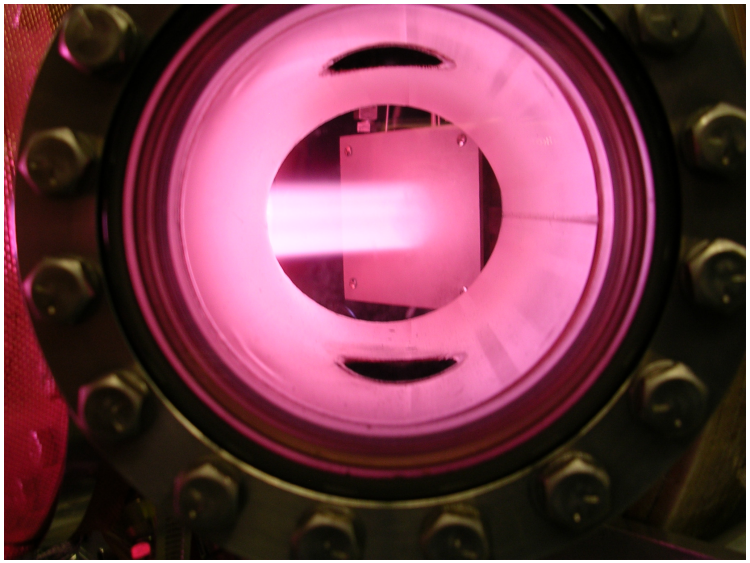


- **Adding small amount of Ar to D plasma increases sputtering yield even though $Y_{DonBe} > Y_{AronBe}$ @ 100 eV**
- **Macroscopic morphology (SEM) is different, but no substantial difference in nanoscopic (TEM) surface features**
- **Thin (5-10 nm) amorphous-like surface layer exists in both cases**

Cambridge Laboratory for Accelerator-based Studies of Surfaces (CLASS)



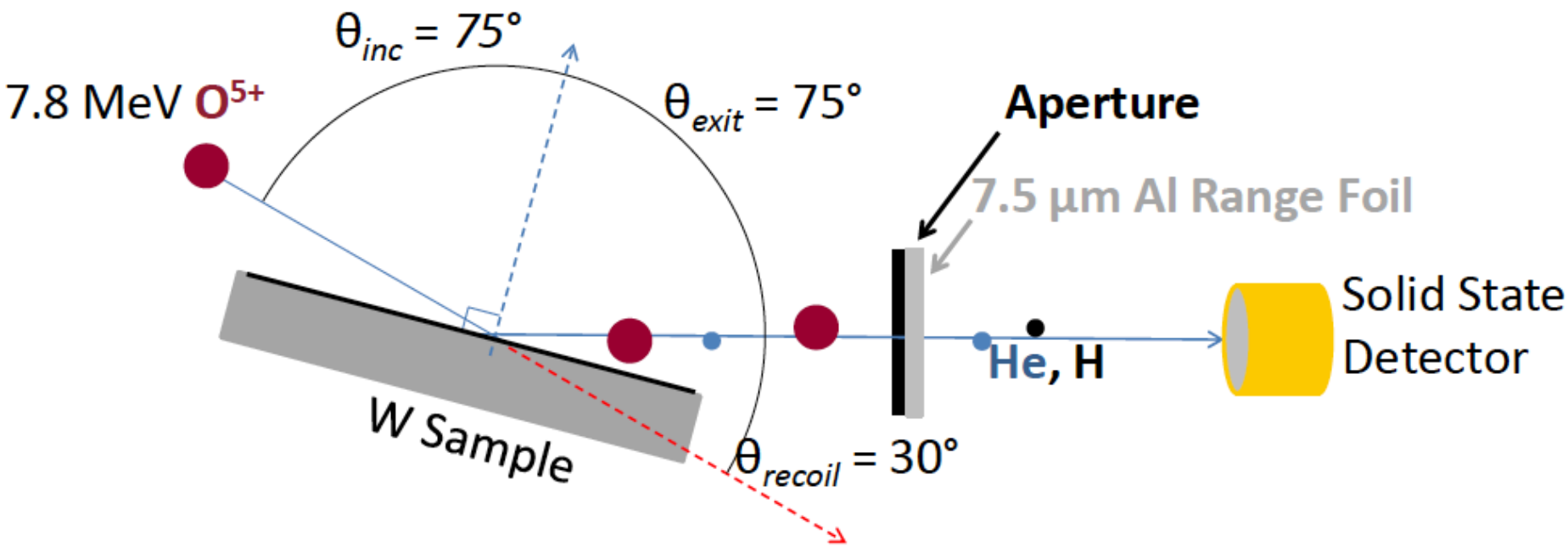
1.7 MV Cockcroft-Walton tandem accelerator



DIONISOS Experiment

- CLASS is part of the DoE-funded PSI Science Center of Excellence in collaboration with UCSD, U of Tennessee, SNL, and INL.
- Work is mostly on fusion materials but there are active collaborations in other fields:
  - Tungsten fuzz growth
  - Diagnostic development (RFQ, ion-sensitive probes)
  - Material erosion in plasma thrusters
  - Post-mortem material analysis for tokamak surfaces

How to measure spatially resolved He concentration in W?

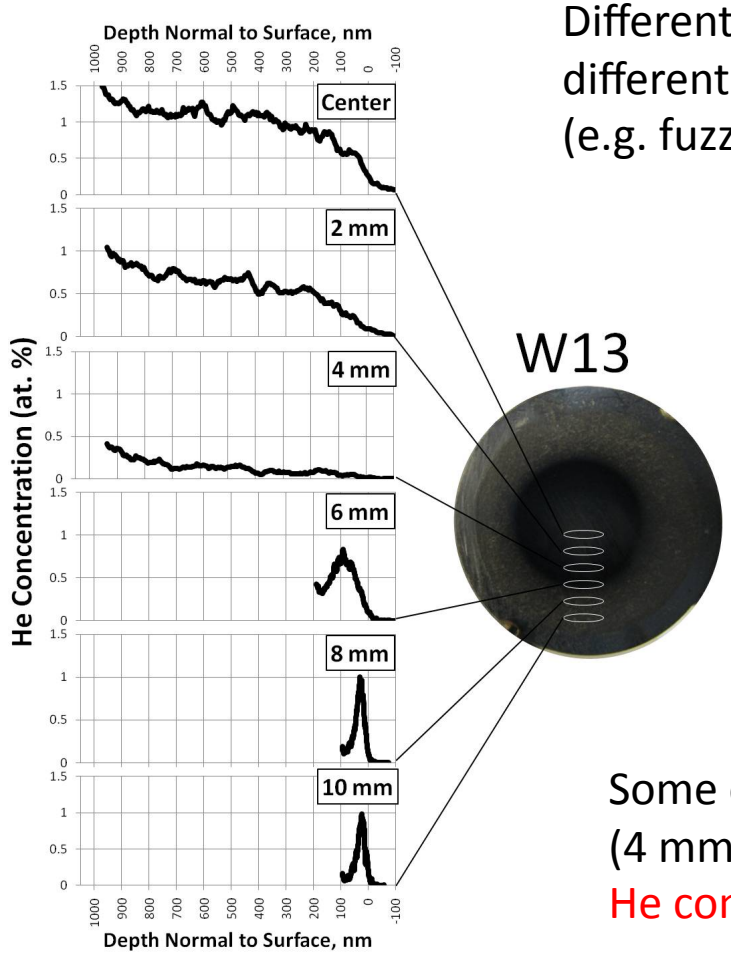


- Heavy-ion (O^{5+}) elastic recoil detection (ERD) gives the He concentration depth profile in the near surface.
- ~1 mm oblong beam spot gives decent spatial resolution.
- Limited range of ERD is somewhat off-set by porosity of W “fuzz”

He concentration in fuzz layer

The He concentration is constant throughout the entire fuzz layer but strongly peaked at the surface for pre-fuzz conditions

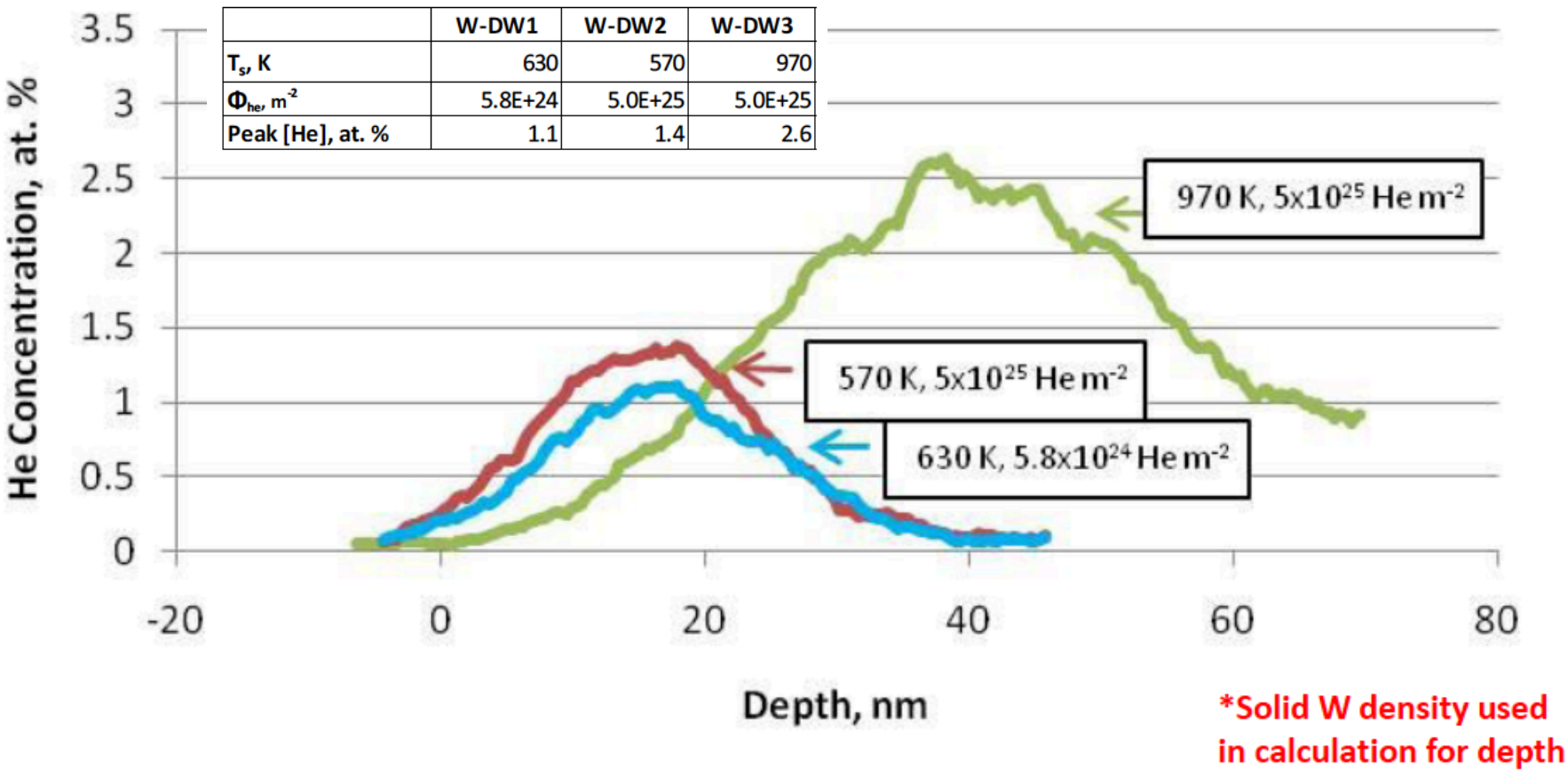
	T_s [K]	Φ_{He} [10^{24} ions m^{-2}]
W Fuzz	1470	670
	1290	530
	1150	315
Pre-Fuzz	1010	140
	920	53
	750	8



Different depth scales correspond to different assumptions on W density (e.g. fuzz layer ~10 % bulk density)

Some of the early stage fuzz growth (4 mm, 2 mm) may indicate lower He concentration in early growth.

How much He can tungsten trap? What are the controlling parameters?



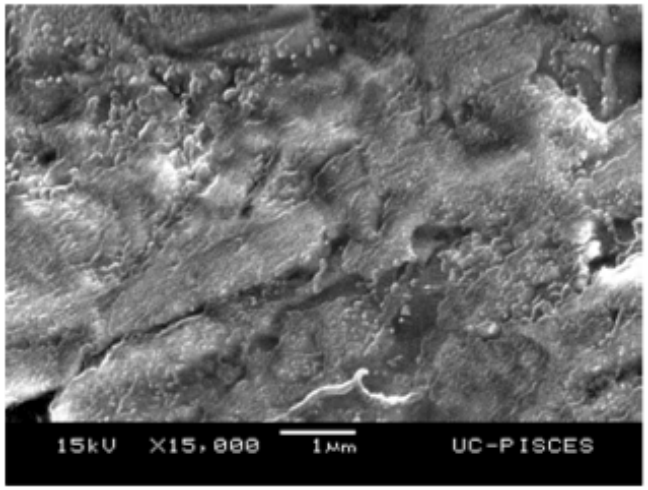
	W-DW1	W-DW2	W-DW3
T_s, K	630	570	970
Φ_{he}, m^{-2}	5.8E+24	5.0E+25	5.0E+25
Peak [He], at. %	1.1	1.4	2.6

*Solid W density used in calculation for depth

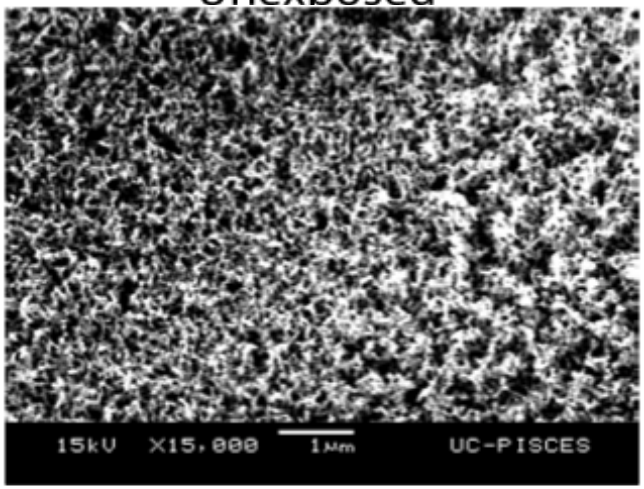
- None of these targets show signs of fuzz growth (by eye)
- Higher local concentrations of He at high T_{surf} and deeper diffusion.
  - Lower surface conc. may be bubbles reconnecting to the surface and breaking open.

Can fuzz form in ITER and reactors?

- **Linear plasma device like PISCES have grown micron-thick nano-tendril or "fuzz" layers from metallic Mo/W surfaces**
- **Recipe: Low-energy Helium ions + $T_{surface}$ ~900-1400 K**
- **These conditions are expected in ITER and reactor divertors.**
- **However, fuzz never documented in tokamak divertor which has large differences to linear plasmas**
  - **Grazing magnetic field vs. perpendicular**
  - **Transient vs. steady-state**
  - **Short ionization MFP & fluid-like transport vs. weak ionization & recycling.**
- **Exploit ITER/reactor similar C-Mod divertor**
  - **High heat flux, ITER density, Mo metal surfaces**



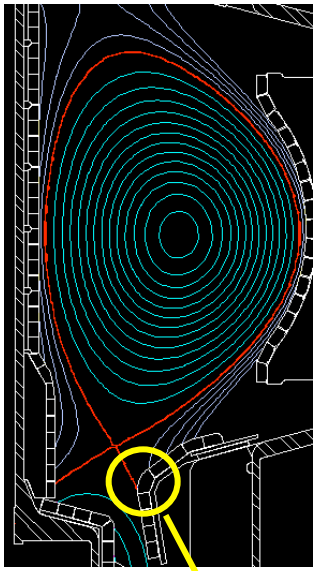
Unexposed



Exposed

Tungsten "fuzz" made in PISCES
T_{surf} ~ 1100 K

He plasmas in Alcator C-Mod produce conditions for fuzz growth at the outer strikepoint



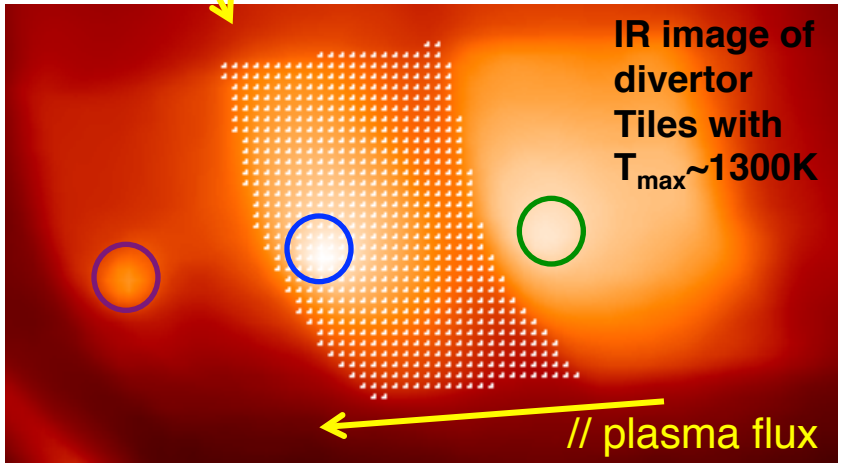
12 shots, ~ 3 MW ICRF, L-Mode

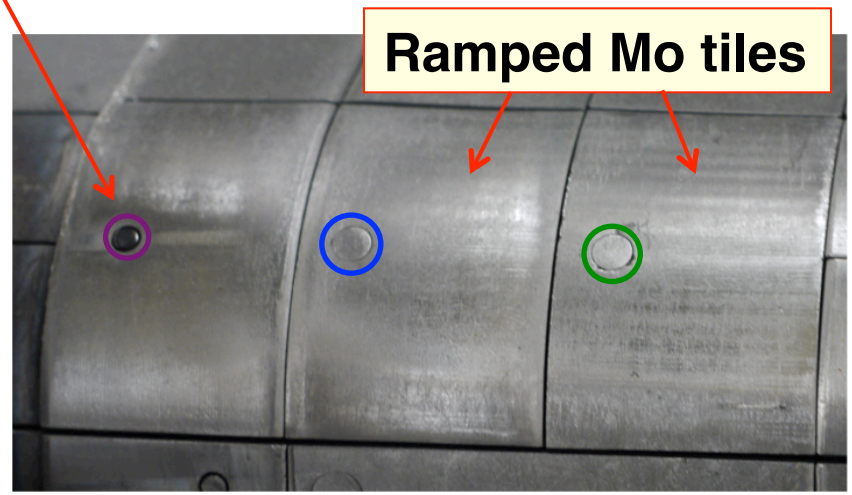
$T_{e,divertor}$ ~ 20 eV, $q_{//}$ > 0.2 GW/m^2

~ 12-15 seconds exposure

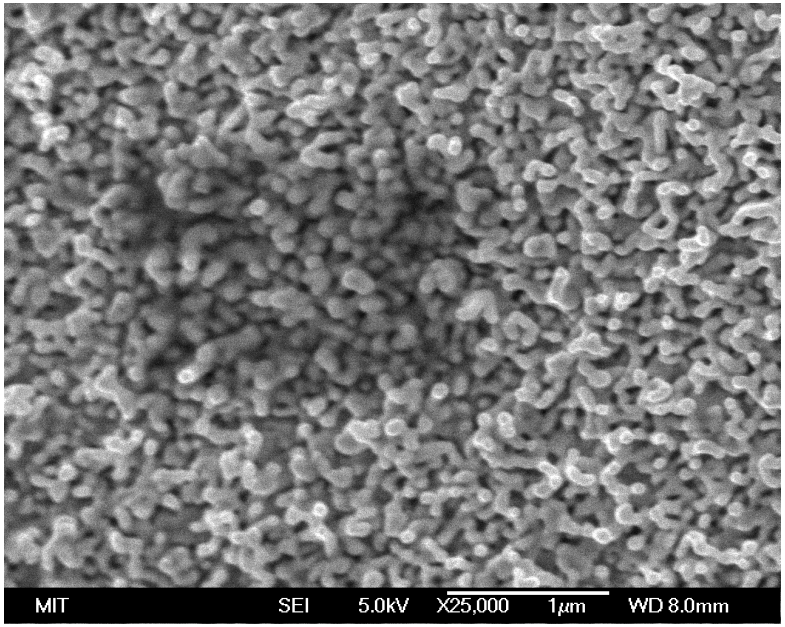
W langmuir probe and Mo calorimeters were hottest

Clearly reduced reflectivity of W probe indicative of fuzz



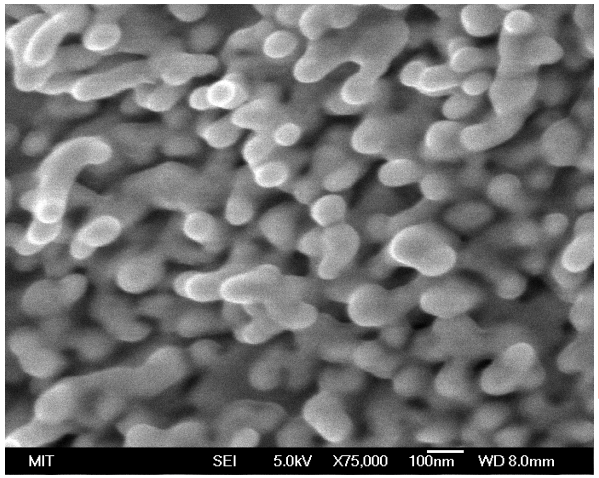


SEM imaging shows nano-tendrils on tungsten probe surface

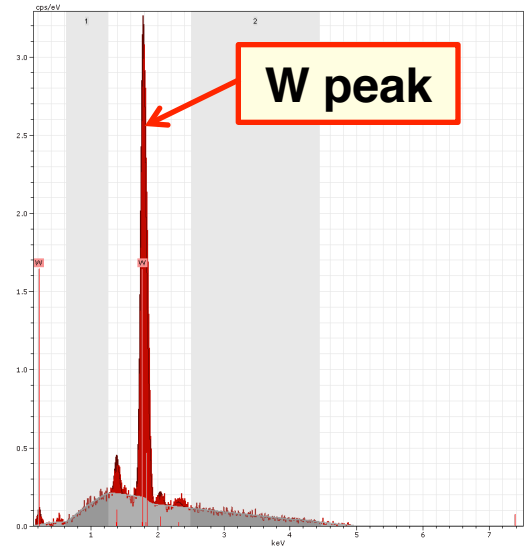


Fully formed nano-tendrils have almost total surface coverage of the probe tip.

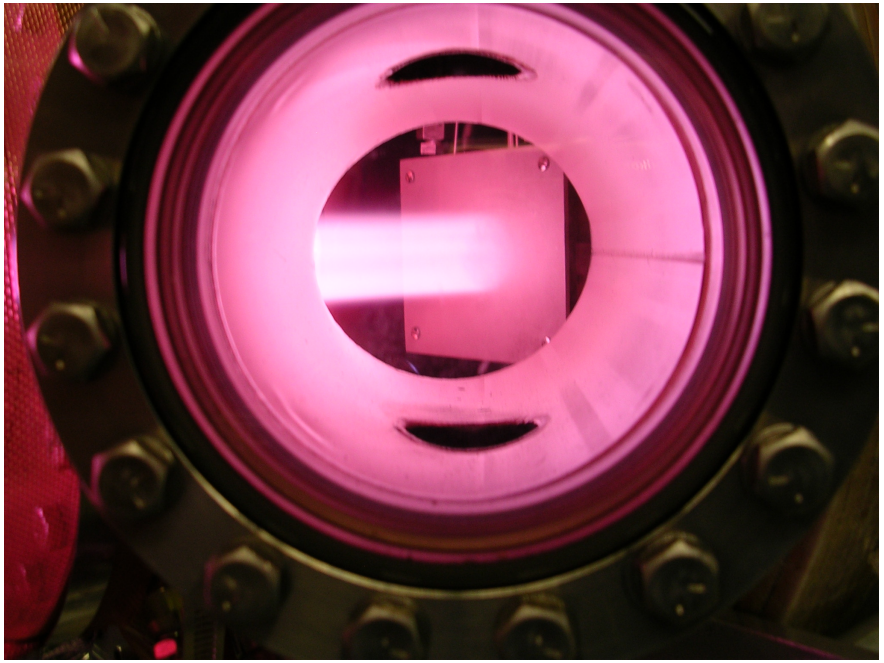
EDX measurements confirm that the fuzz is ~100 % tungsten.

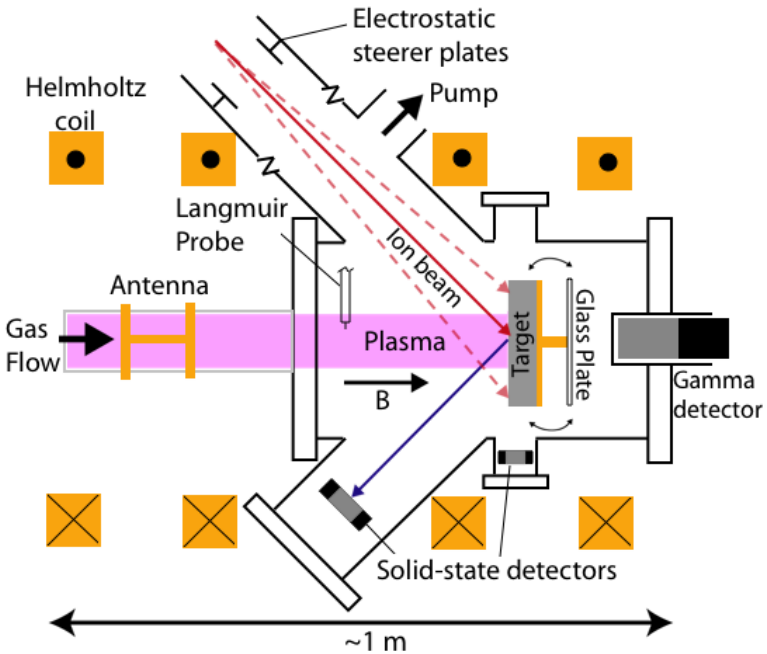


Thickness of individual tendril is 50-100 nm, which is thicker than tendrils grown in linear devices (20-30 nm)



Unique capabilities of DIONISOS

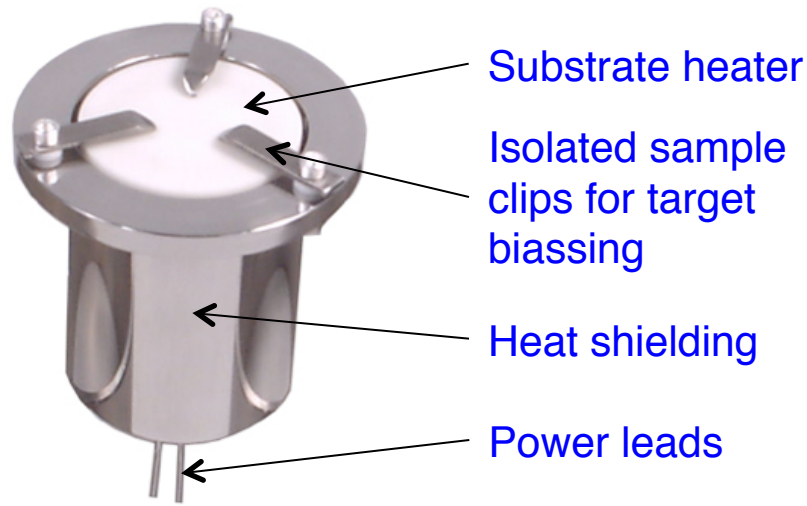




- Simultaneous plasma and ion beam exposure of targets
- Active target heating and cooling (T_{target} = 300-750 K)
- In-situ, *time-resolved* ion beam analysis
- In-situ target irradiation by high-energy (~MeV) ions for irradiated materials studies.

DIONISOS has plasma capabilities & target heater to grow fuzz

	DIONISOS (MIT)
Deuterium ion flux ($m^{-2}s^{-1}$)	10^{20}-10^{22}
Ion energy (eV)	20-350 (bias)
T_e (eV)	5-10
T_i (eV)	2 - 5
n_e (m^{-3})	10^{17}-10^{19}
P_{max} (MW/m^2)	0.6
Plasma diameter (mm)	50
Pulse length (s)	Steady-state
Activated targets	No
Tritium	No

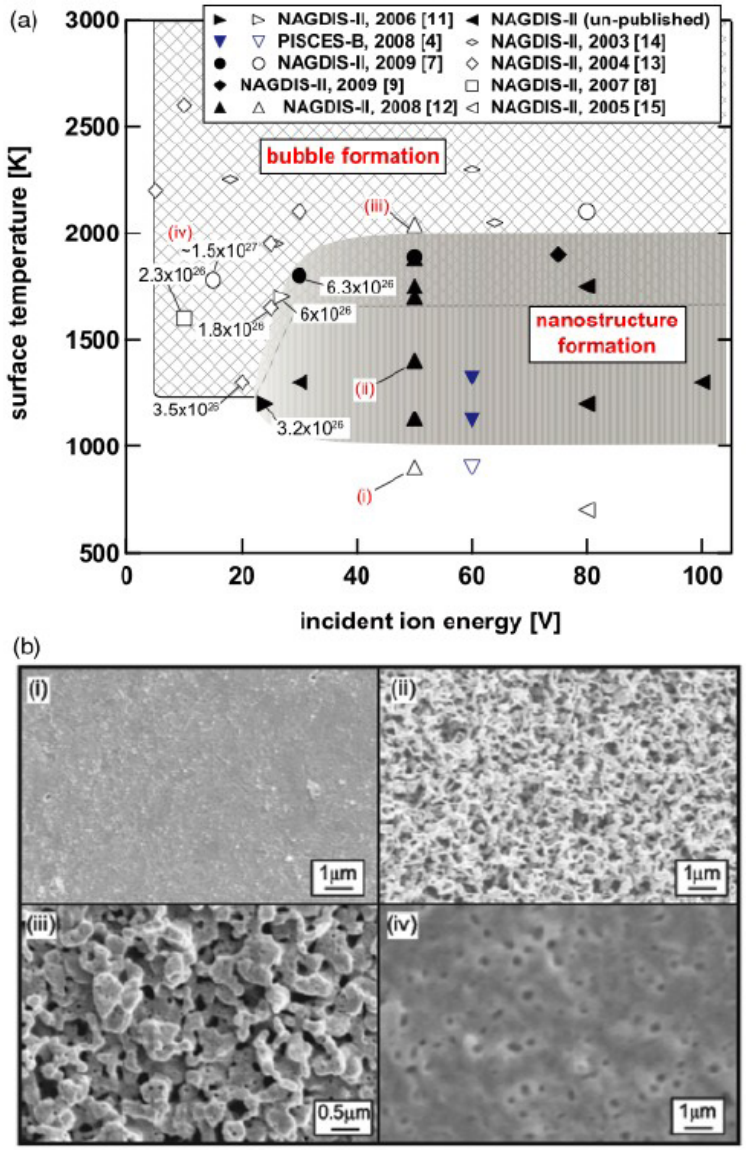


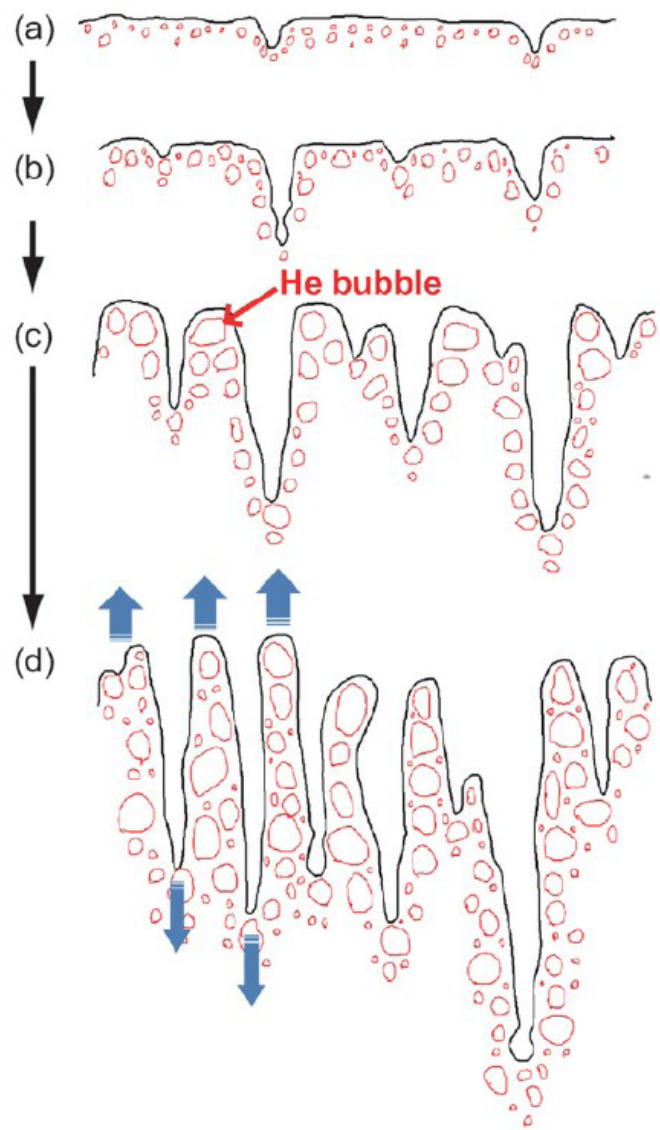
- T_{MAX} ~ 1473 K
- Electrically isolated from target
- Mo heat shielding

In-situ ERD allows for the He concentration to be measured in-situ during fuzz growth.

*Proposed W fuzz formation mechanism**

- **Sub surface He bubbles drive 'finger' instability**





* Kajita, *Nuclear Fusion* **49** (2009) 095005.

*Proposed W fuzz formation mechanism**

- **W 'viscosity' drives transport from below bubble layer driving fuzz growth**

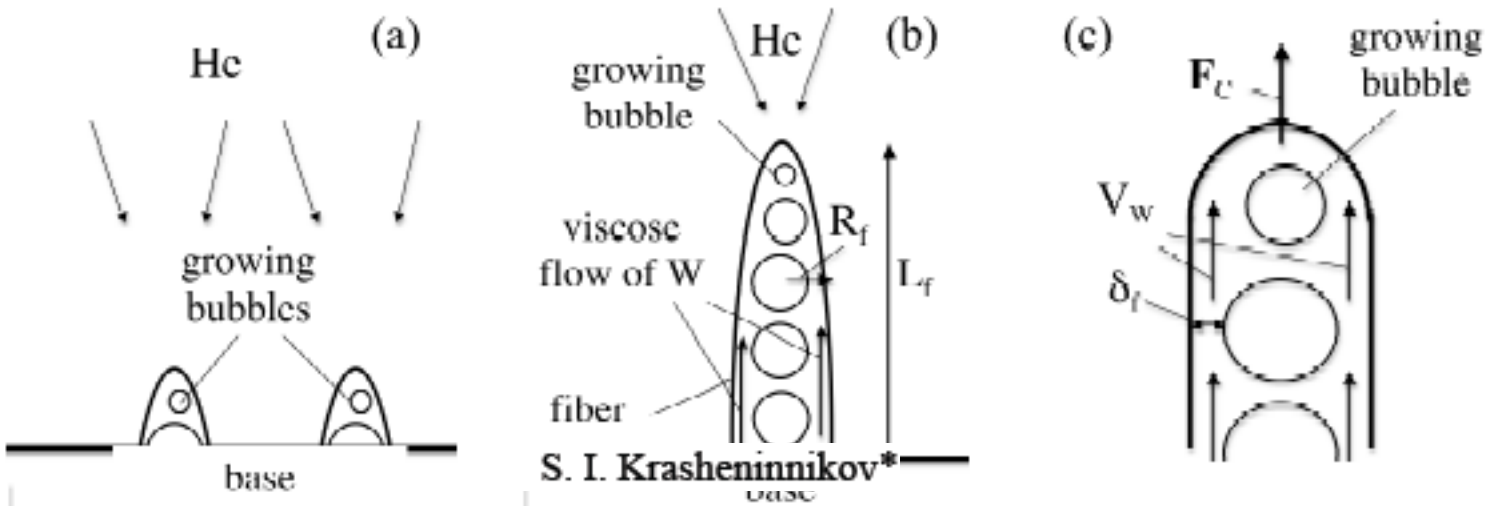


Fig. 2. Schematic views of: (a) initial stage of the fiber growth; (b) developed fiber; (c) viscose flow of W to the tip of the fiber due to the force caused by the pressure of the He in the growing fiber.

$$F_C = P_{He}\pi R_f^2, \tag{2}$$

where P_{He} is the helium pressure in the bubble of radius R_f, which we will assume to be large the thickness of the fiber "skin", δ_f. Helium pressure in the growing bubble can be estimated as

$$P_{He} \sim 2\gamma / R_f, \tag{3}$$

where γ is the tungsten surface tension coefficient.

As a result, the magnitude of the stress in the "skin" can be evaluated as

$$\sigma_0 \sim \frac{F_C}{2\pi R_f \delta_f} \sim \frac{2\gamma}{2\delta_f}. \tag{4}$$

Then substituting expression (4) in Eq. (1) we have

$$\frac{\partial \sigma_{\ell\ell}}{\partial \ell} \sim \frac{\sigma_0}{L_f} = \mu_W \frac{V_W}{\delta_f^2}, \tag{5}$$

where L_f is the length of the fiber and V_W is the flow velocity of tungsten (see Fig. 2c). Then taking into account that $dL_f/dt = V_W$ from Eq. (5) we find:

$$L_f(t) = \sqrt{\frac{2\gamma\delta_f}{\mu_W} t}. \tag{6}$$

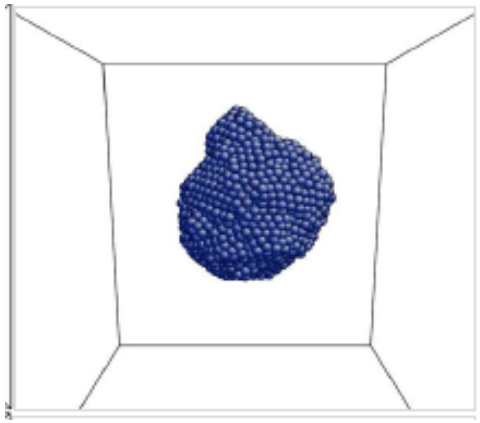
* Krasheninnikov, (2011) manuscript in preparation.

MD simulations: sub-surface He bubbles

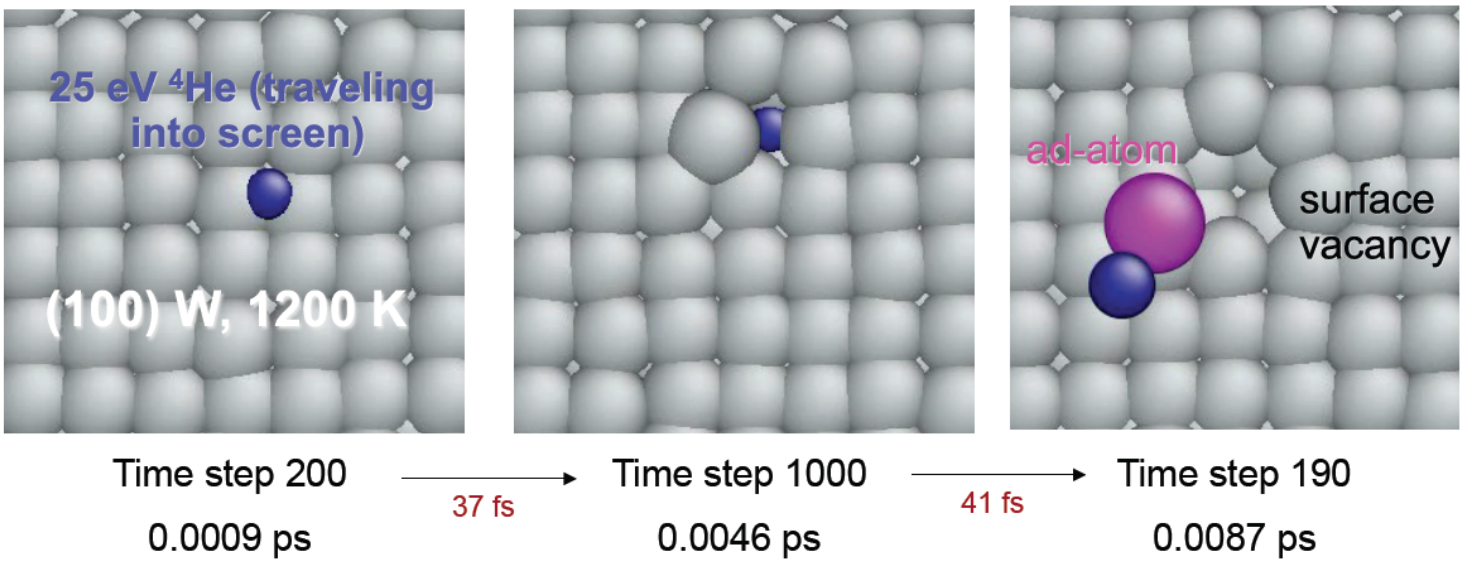
• Evolution of He bubbles below surface: initial nucleation & growth require a kinetic model (in progress)

• Evolution of larger He bubbles -> several regimes of interest:

- Equilibrium bubbles (internal gas pressure $P = 2\gamma/R$)
- Over-pressurized bubbles can 'punch loops' ($P = 2\gamma/R + Gb/R$)
- Near-surface, over-pressurized bubbles can rupture



How do these processes influence surface topology evolution, sputtering, etc. & can sub-sputtering threshold He exposure drive surface evolution processes?



Pressure evolution of He bubbles

Molecular dynamics simulations to assess He bubble pressure & response of over-pressurized, sub-surface bubbles (R ≈ 1.6 nm)

- Equilibrium bubble and loop punching

Ackland-Thetford W-W, Henriksson W-He, Beck He-He
Future studies with other potentials

Equation of state *(Wolfer 1988)*

R=5 a_0 1044 W vacancies

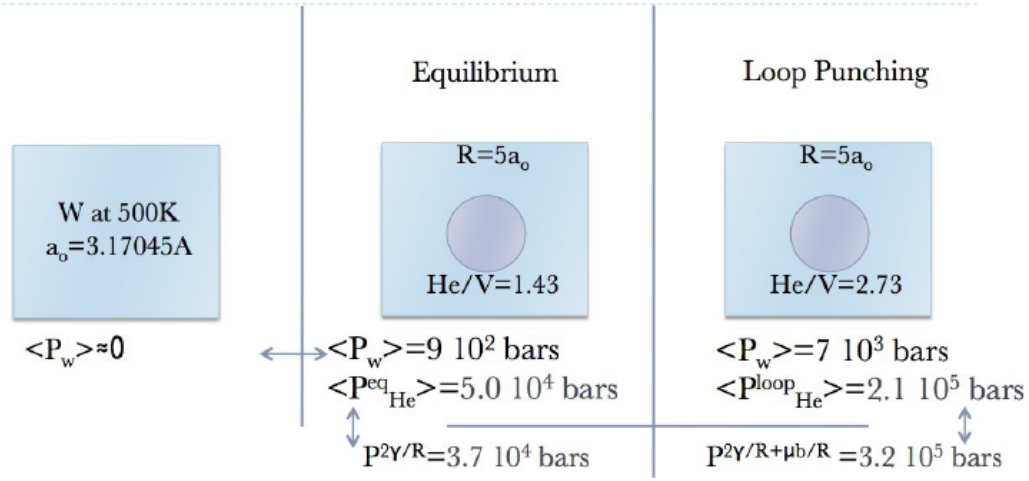
$P_{eq} = \gamma / 2R$

Temperature (K)	500	1200	2000
# He in bubble	1 497	1 234	998
He/V ratio	1.43	1.18	0.969

$P_{loop} = \gamma / 2R + \mu\, b/R$

Temperature (K)	500	1200	2000
# He in bubble	2 847	2 754	2 610
He/V ratio	2.73	2.65	2.53

PBC results at T=500K



- # He is derived from the EOS of He using $P_{eq} = 2\gamma / R$ and $P_{loop} = \frac{2\gamma}{R} + \frac{\mu b}{R}$

γ : surface tension
R: radius of bubble
b: burger's vector
μ : shear modulus

- Compute pressure of He in bubble, P_{bubble}, and pressure of W in the bulk P_{bulk}
- Compare P_{bubble} and $P_{eq} = 2\gamma / R$ and then with $P_{loop} = \frac{2\gamma}{R} + \frac{\mu b}{R}$
- Compare P_{bulk} and P_w

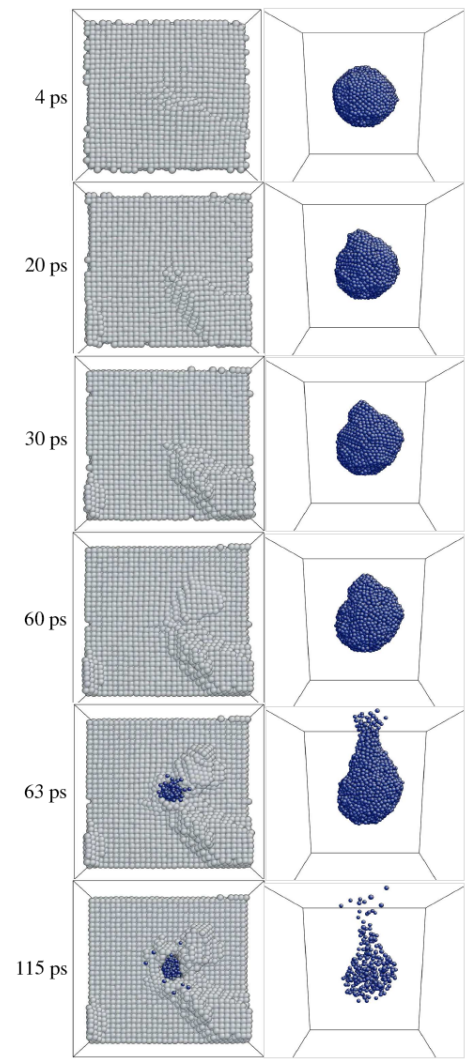
Pressure evolution of He bubbles

- He bubble close to the surface will burst if the pressure is “too high”
  - lead to cratering but no W erosion observed (MD timescales)
- Dependent on distance below surface, size, P, T

Bubble stability as a function of d, depth

He/V	1.43	2.74	3.07	3.85	4.08
$d = a_0$	bursts				
$d = 2\ a_0$	stable	bursts			
$d = 3\ a_0$		stable	bursts		
$d = 5\ a_0$			stable	bursts	
$d = 10\ a_0$				stable	stable

- $d < R \rightarrow$ bubble bursts for He/V < He/V^{loop}
- $d = R = 5\ a_o$:
  Number of He for $P^{2\gamma/R+\mu b/R}$ is 3787 and He/V=3.63
  Number of He for bursting is 4025 and He/V=3.85
  (4025-3727)/3727 = 6% discrepancy in number of heliums between loop punching pressure and bubble bursting
- $d = 2\ R = 10\ a_0 \rightarrow$ bulk behavior (no surface effect)

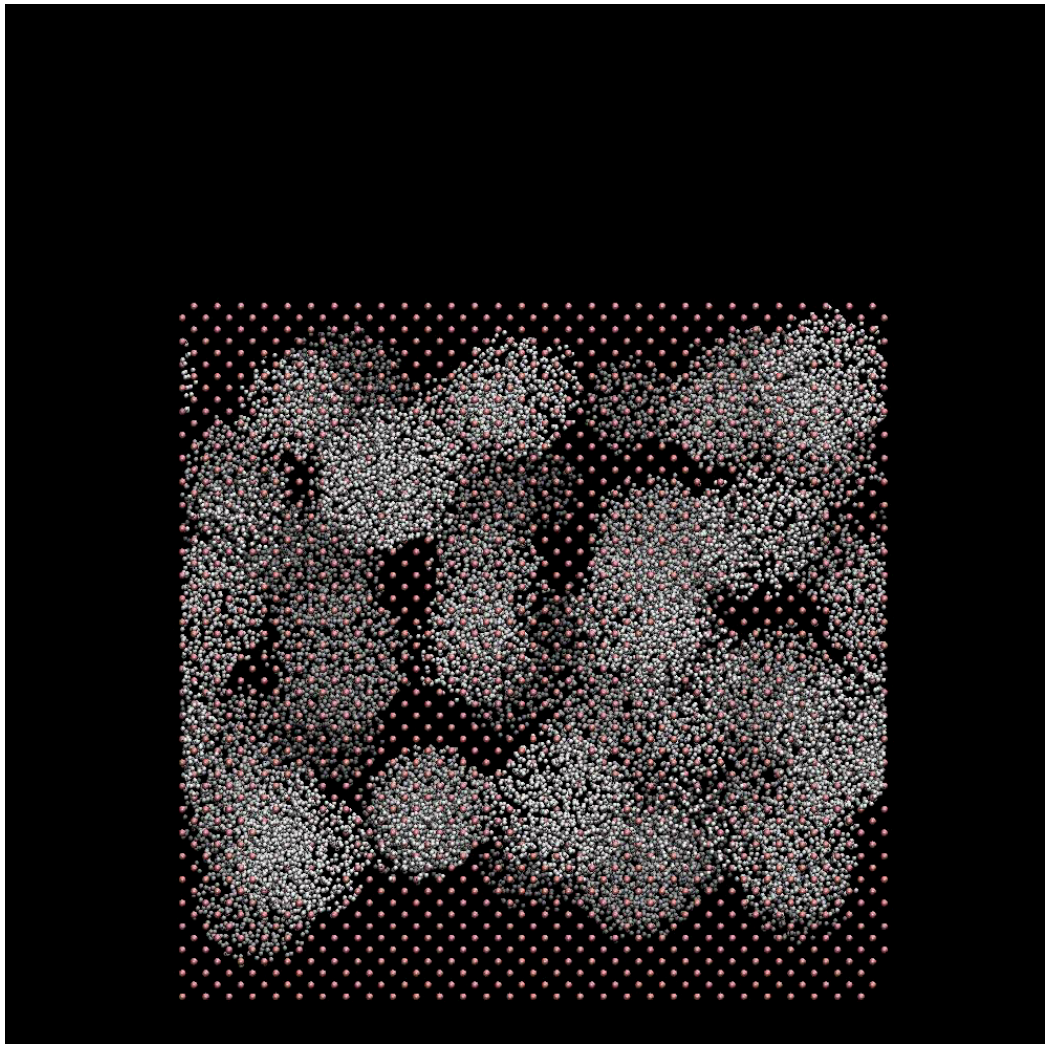


movie

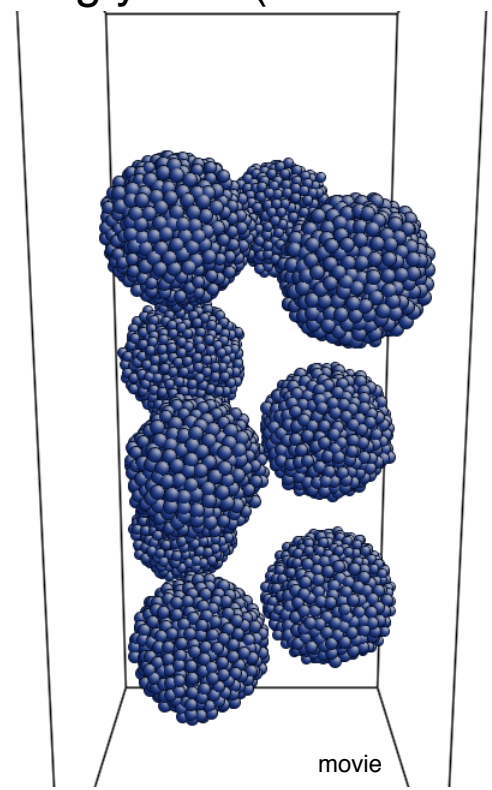
He bubble influence on sputtering & evolution

- How do sub-surface He bubble influence sputtering?
- How do sub-surface He bubbles grow to drive burst phenomena

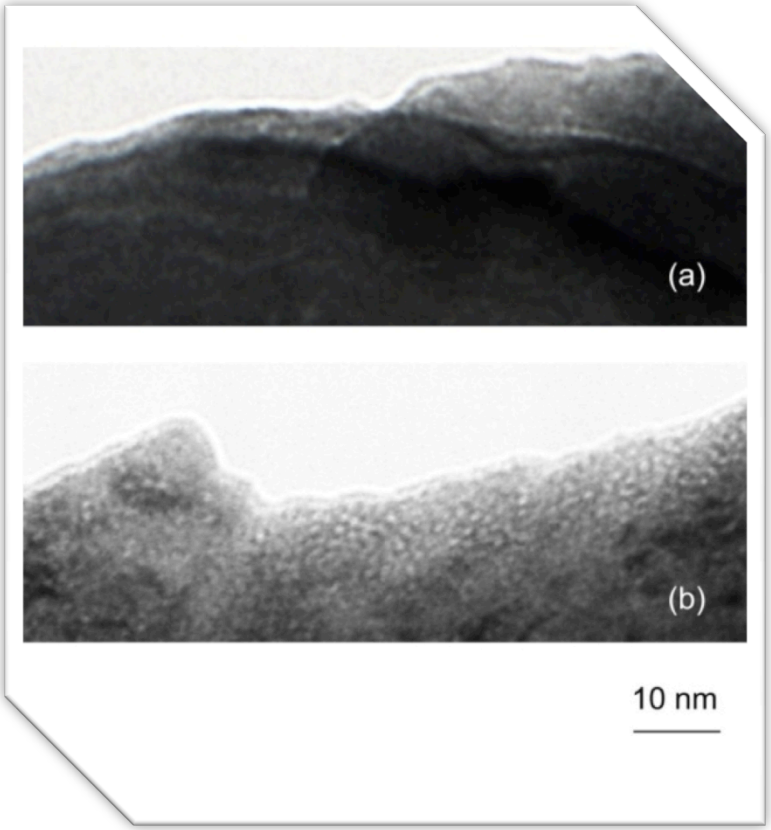
MD of evolution of He bubble population at 600K
R ~ 0.9 ± 0.5 nm, 2 He/V, d > 0.3 nm



9 bubbles inserted d > 1.6 nm below (100) W surface, 1.2 < R < 1.4 nm, P = 2γ/R
15% He bubble fraction
- Evaluate He induced sputtering yields (300-600 eV)



Role of near-surface bubbles on tungsten erosion



- **W exposed to low flux He plasma (a) does not result in He nano-bubble formation (UCSD)**
- **Higher flux He plasma (b) does cause He bubble precipitation (UCSD)**
- **Ion beam sputtering of both type of surfaces (a & b) shows no clear difference (IPP-Garching)**
- **Simultaneous sputtering and gas concentration depth profile measurements in DIONISIS (MIT) are being discussed**
- **MD modeling of sputtering from surfaces with voids being performed (U. Tenn.)**

PSI Science Center Summary & Future Efforts

- **Multi-institution PSI Science Center with goal of interdisciplinary science investigation of plasma surface interactions involving exposure, (in-situ) diagnostics and modeling**

- **Tungsten fuzz formation mechanism remains unresolved –**
  - **Key observation that it is not only a laboratory observation**
  - **Continuing to work toward models to predict fuzz formation & the critical steps in nucleating the growth of fuzz**

- **Continued coordinated efforts on W fuzz formation & the role of sub-surface He bubbles on W sputtering yields do to He ion irradiation**