Overview of the UC San Diego PISCES Program

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U.S. MFE Structural Materials &
Plasma-Materials Interaction Workshop
UT-Knoxville & ORNL

July 25-29, 2016

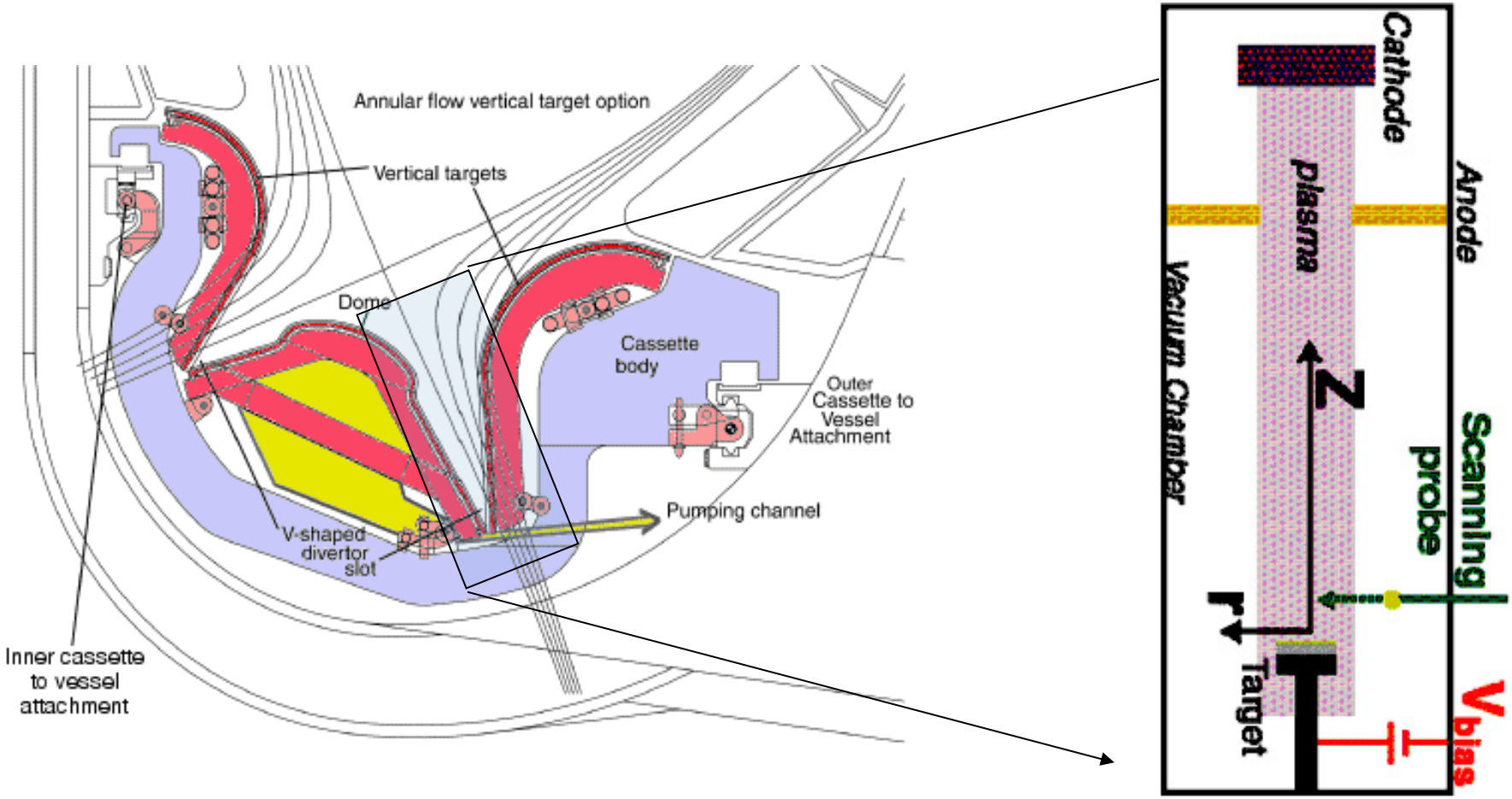
PISCES Program Goal:

Carry out Basic Plasma-Materials Interaction & Boundary Plasma Experimental Science Supporting ***ITER & Fusion Nuclear Science Program***

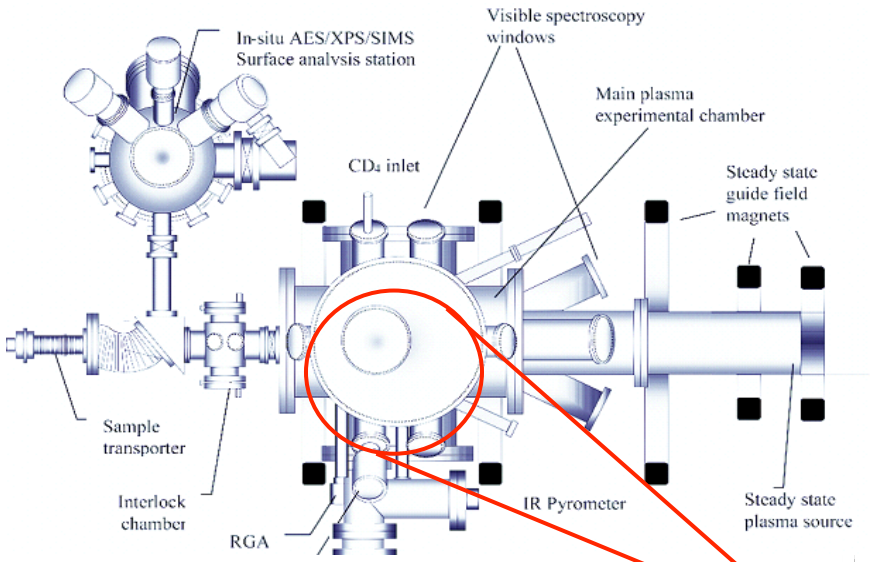
PISCES Program Approach:

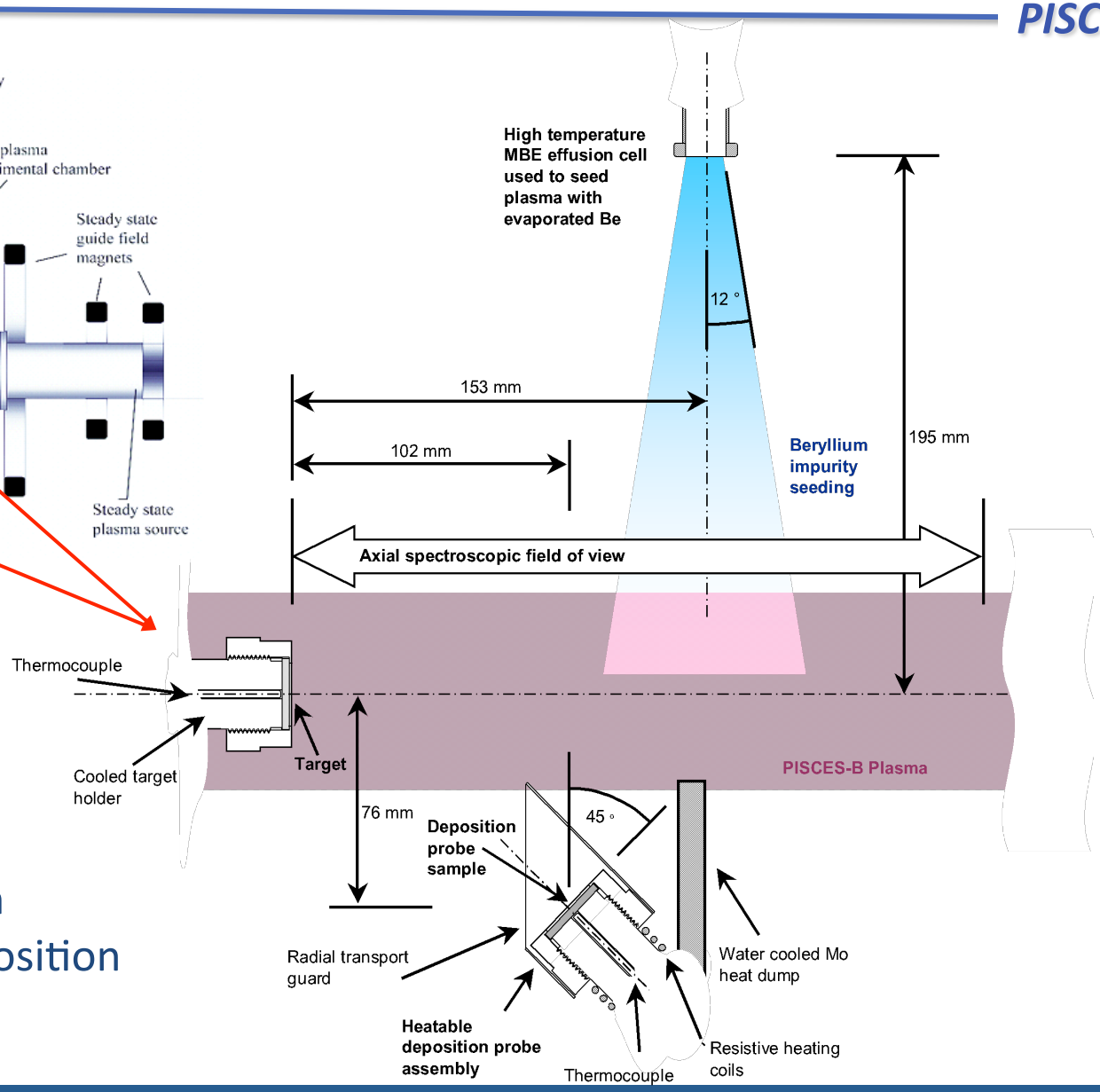
- *Use UNIQUE PISCES & Helicon RF plasma facilities*
- *Extensive collaborations (DIII-D, LHD, Ion Beam Facilities, Modeling)*
- *Develop & Test Hypotheses*
- *Refine Models*
- *Use Validated Models to Project PMI Performance in ITER, DEMO/FNSF conditions*

PISCES Devices Provide a Divertor-like Environment



PISCES-B reproduces materials & conditions found in JET-ILW and ITER

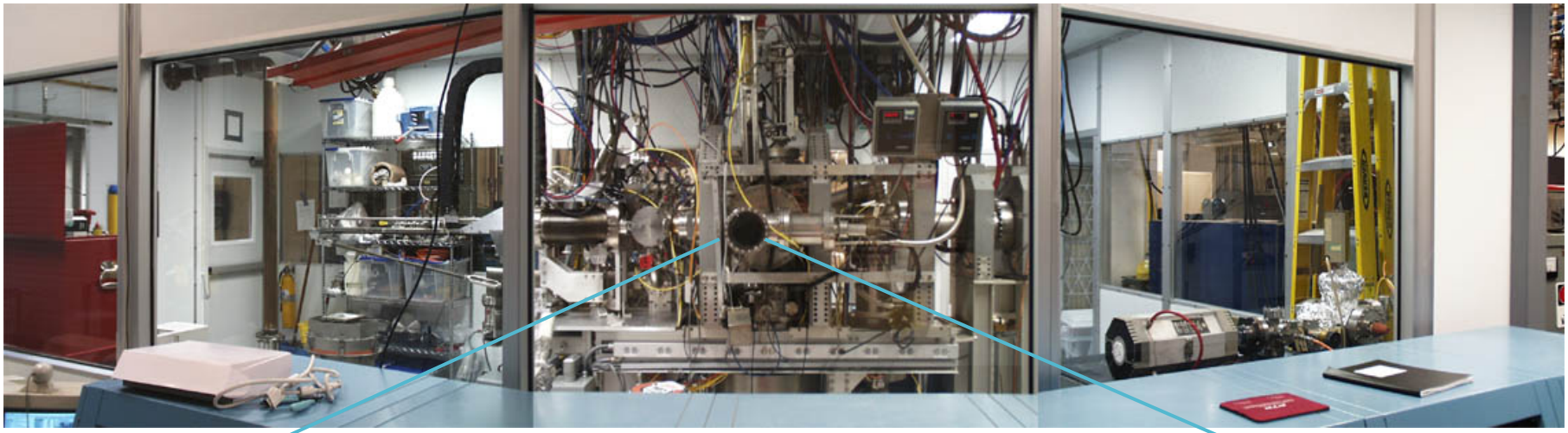


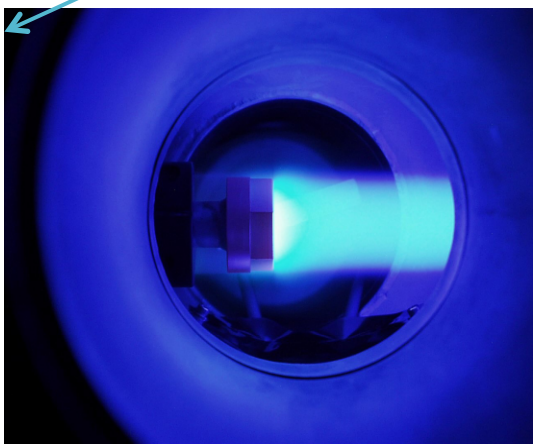


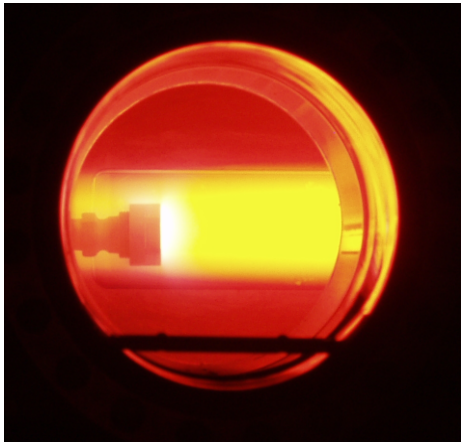
Controlled studies of:

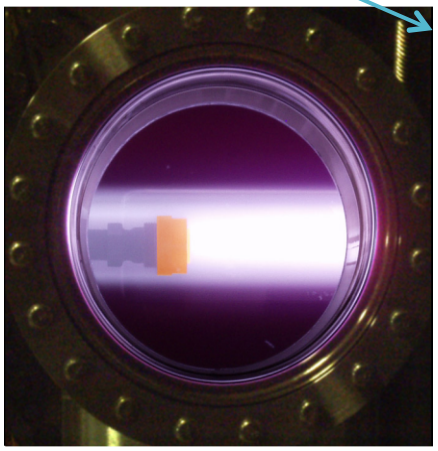
- Be erosion, W erosion
- Morphology evolution
- SOL transport
- Be/W mixed mat'l formation
- D/Be, D/W, D/Be/W Co-deposition
- Thermal transient effects

The PISCES Program Hosts Unique Facilities at UC San Diego





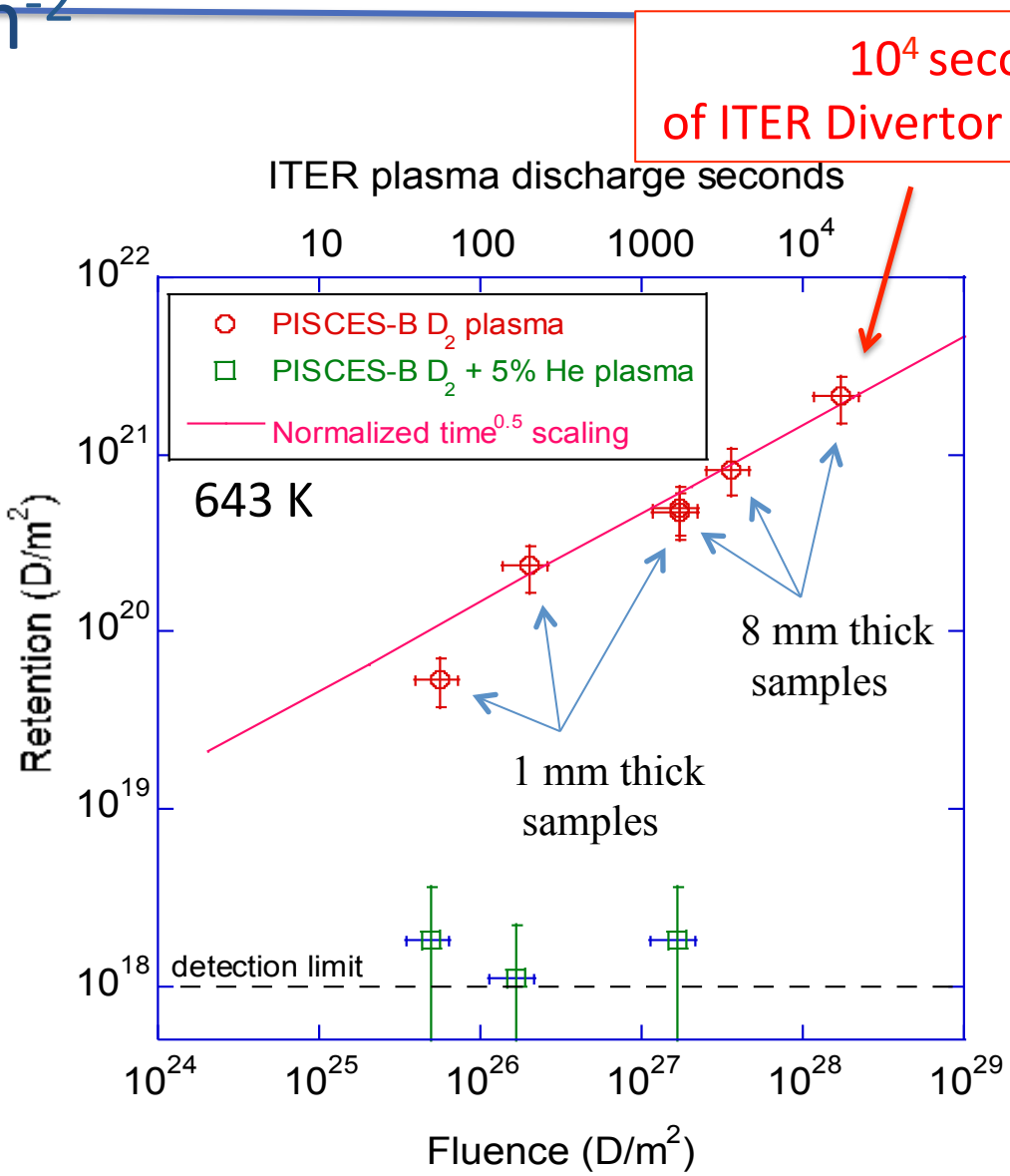




PISCES Supporting ITER PMI Needs

- **Record Fluence Exposures Show No Saturation of D Retention in W**
- He nanobubble formation inhibits D retention in W; similar results observed in Be
- Progress on identifying mechanism of D retention suppressi
- ITER bake studies guide plans for T inventory control
- Discovered workable alternate T inventory control techniqu
- Successful modeling of W-fuzz formation
- Controlled ELM-like thermal transients more clearly define damage thresholds for W divertor target

PISCES-B operated continuously for 31 hours to generate data at a **world-record fluence** of 2 x 10^{28} m^{-2}



- **No saturation in D retention** in W with high-fluence deuterium plasma exposure
- **5% He^+ flux during deuterium plasma exposure drastically reduces D retention** in W at 643 K
- Evidence for a reduction in retention with higher flux, but a systematic study is needed

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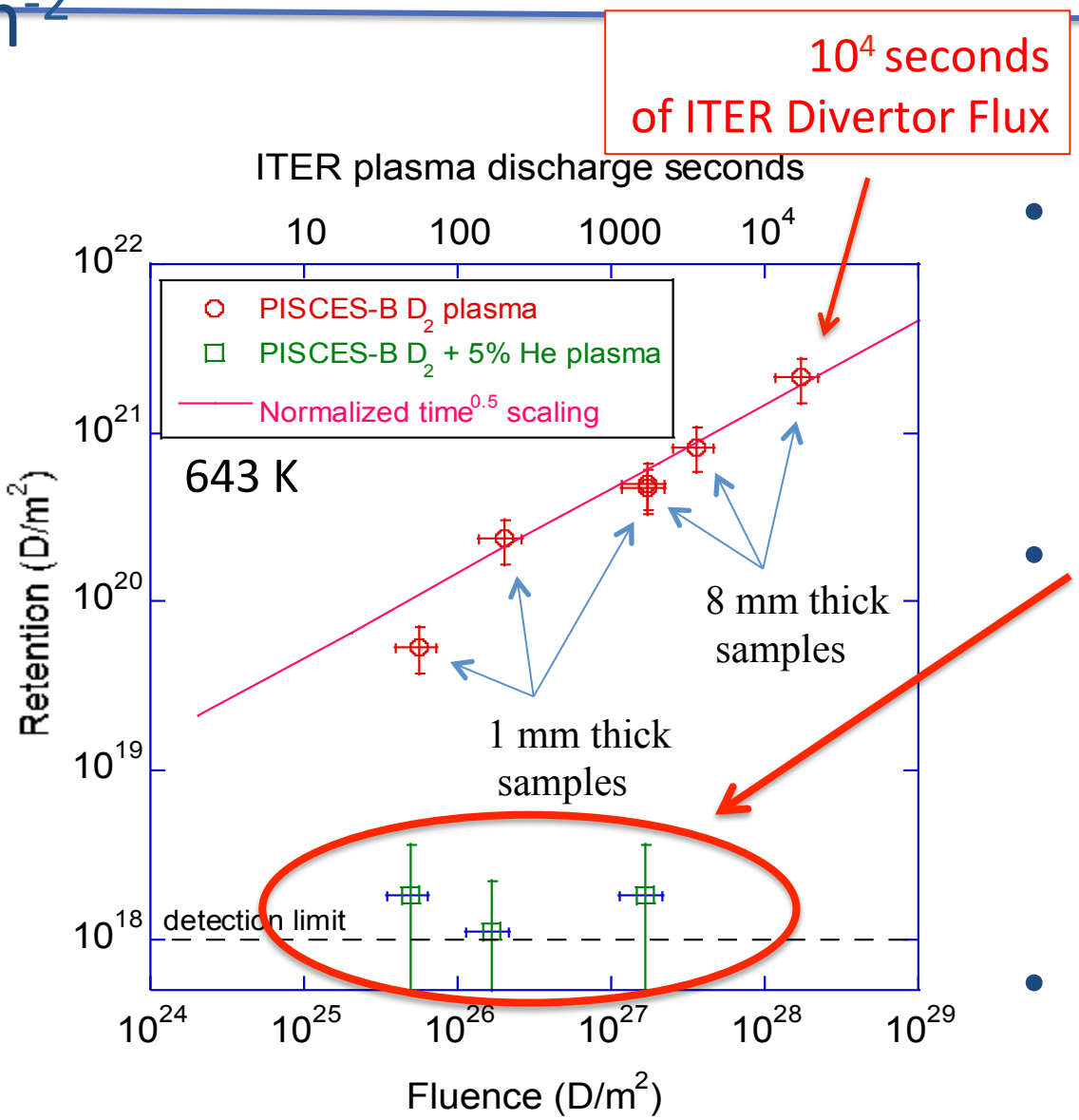

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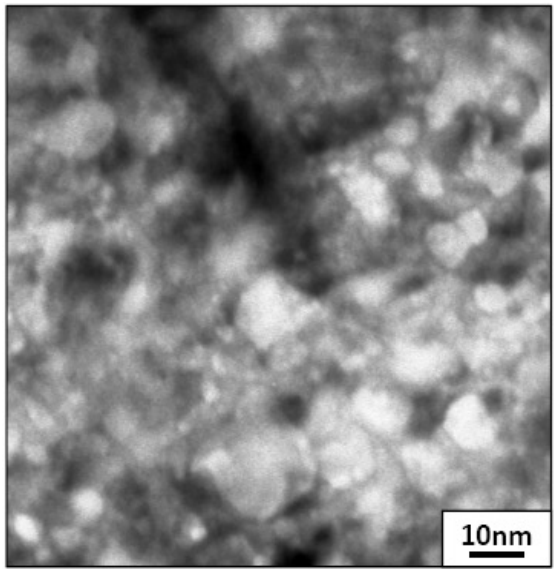
PISCES data helping differentiate between two hypotheses that are proposed to explain reduced D retention due to He

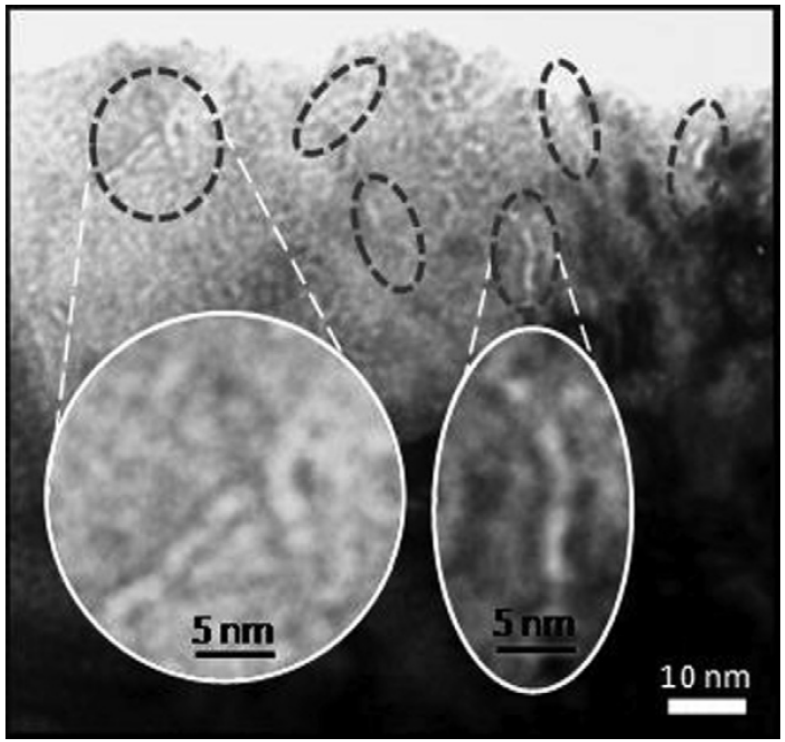
1



TEM image of W sample exposed at ~300°C in P-A to D/He plasma (E_{ion} ~ 60eV) from Miyamoto et a NF 49(2009)065035

- He-filled nano-bubbles close to the surface (20-30 nm) act to trap D atoms
- Migration into the bulk of subsequently implanted D is inhibited

2



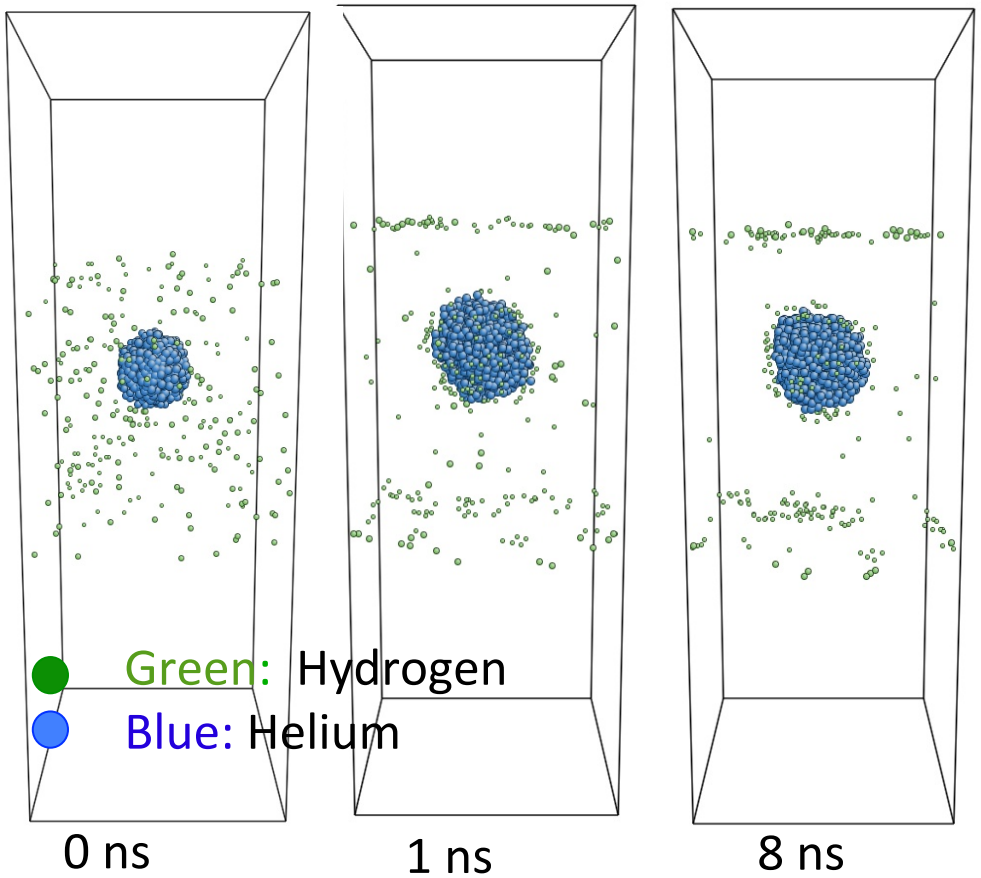
TEM image of W sample exposed at ~500°C in P-A to D/He plasma (E_{ion} ~ 120eV) from Miyamoto et a JNM 415(2011)S657

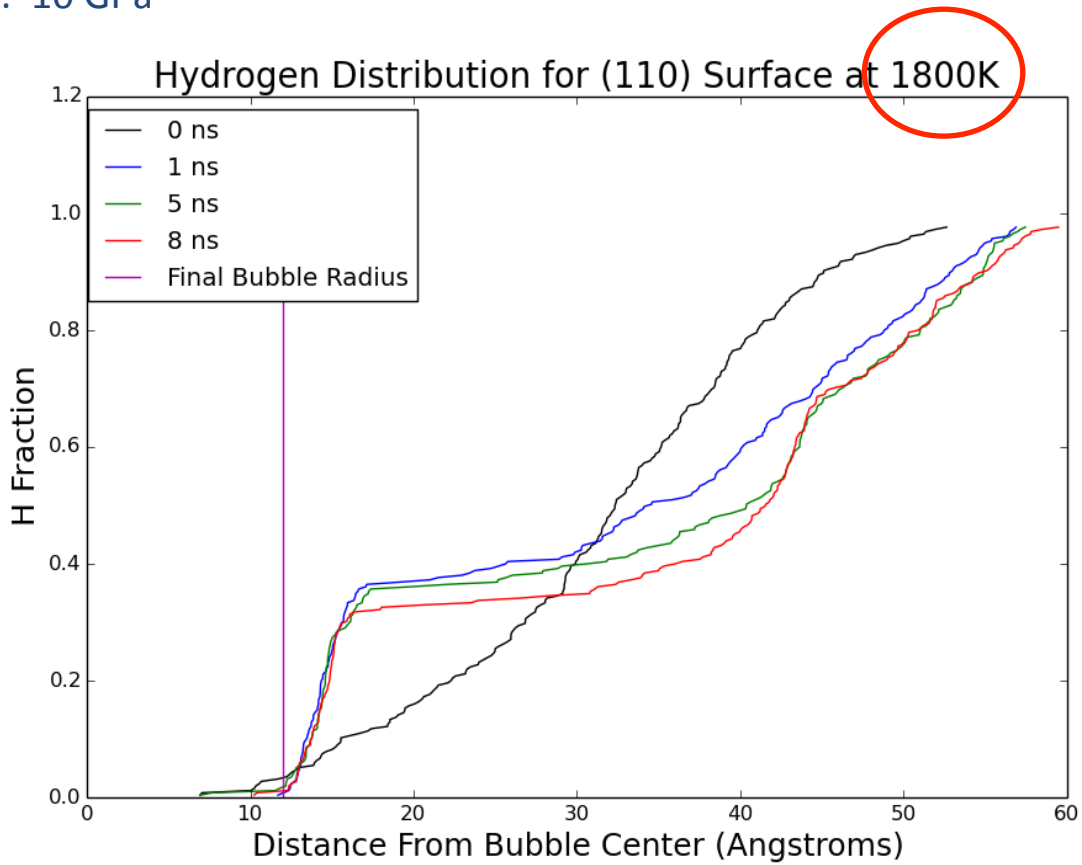
- He nano-bubbles interconnect and reach the surface providing pathways for diffusing D to exit the sample

Preliminary MD results of He-H synergies & H trapping suggest hypothesis ① (courtesy of B. Wirth)

- Initial 2 nm diameter, over-pressurized He bubble created 2 nm below W (110) surface
  - H initially randomly distributed – strong partitioning of H to the bubble surface (~35-40%)

Box Size: 6 nm x 6 nm x 12 nm Initial He Pressure: 10 GPa

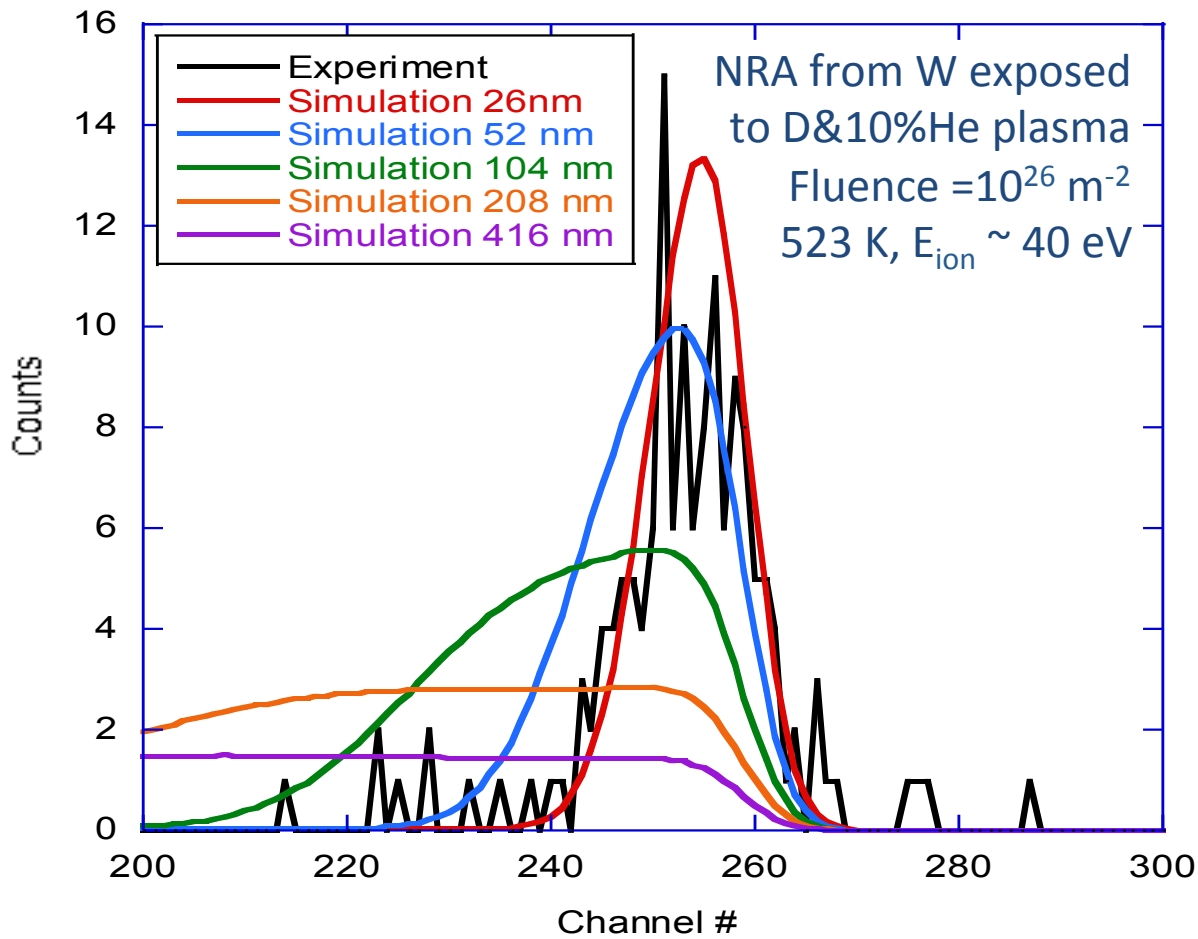




Preliminary modelling of H trapping at He bubbles (or voids) indicates quite strong trapping, with H preferentially located at bubble periphery, even to high temperatures (~2000K) beyond typical TDS measurements – validity of the potentials and extrapolation of these short modeling timescale (~10 nanoseconds) during molecular dynamics simulations are appropriate question to ask.

D partitioning around He bubbles seems to fit NRA experimental data, however, TDS observes release of D

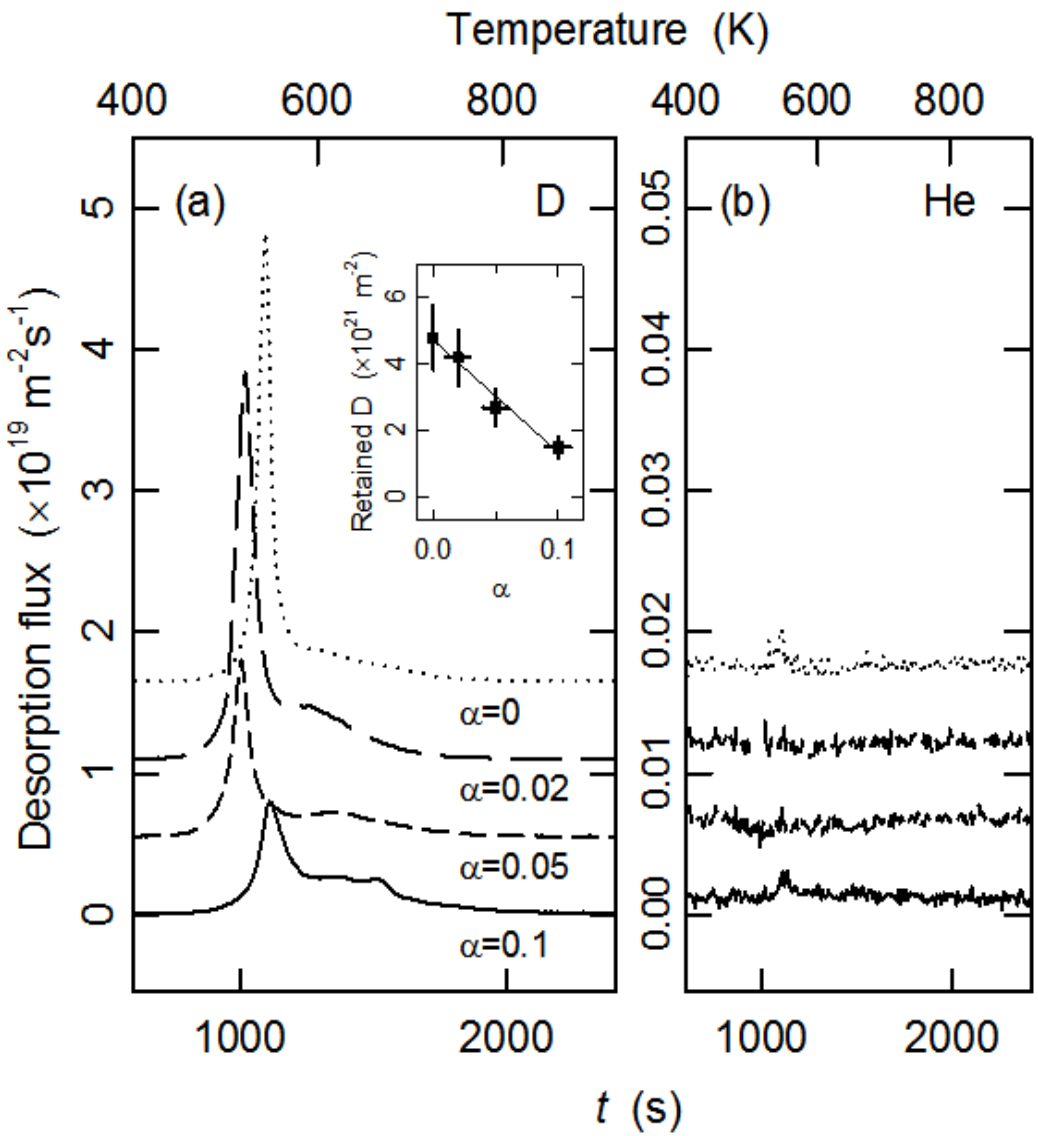
- Location of D retention appears to agree with partitioning around He nanobubbles in agreement with MD simulation
- D is entirely released during TDS in contradiction to MD model (but timescales of TDS and MD simulation are much different, quality of potentials used is also an open question)



Similar D retention reduction observed in Be

- Vary He Concentration Over Different Plasma Exposures
- TDS Emission Spectra
- Results show largest effect in low energy (550 K) release peak

α	**0.0 – 0.1**	
T_{exp}	330	(K)
Φ	1×10^{26}	(m^{-2})
E_i	40	(eV)

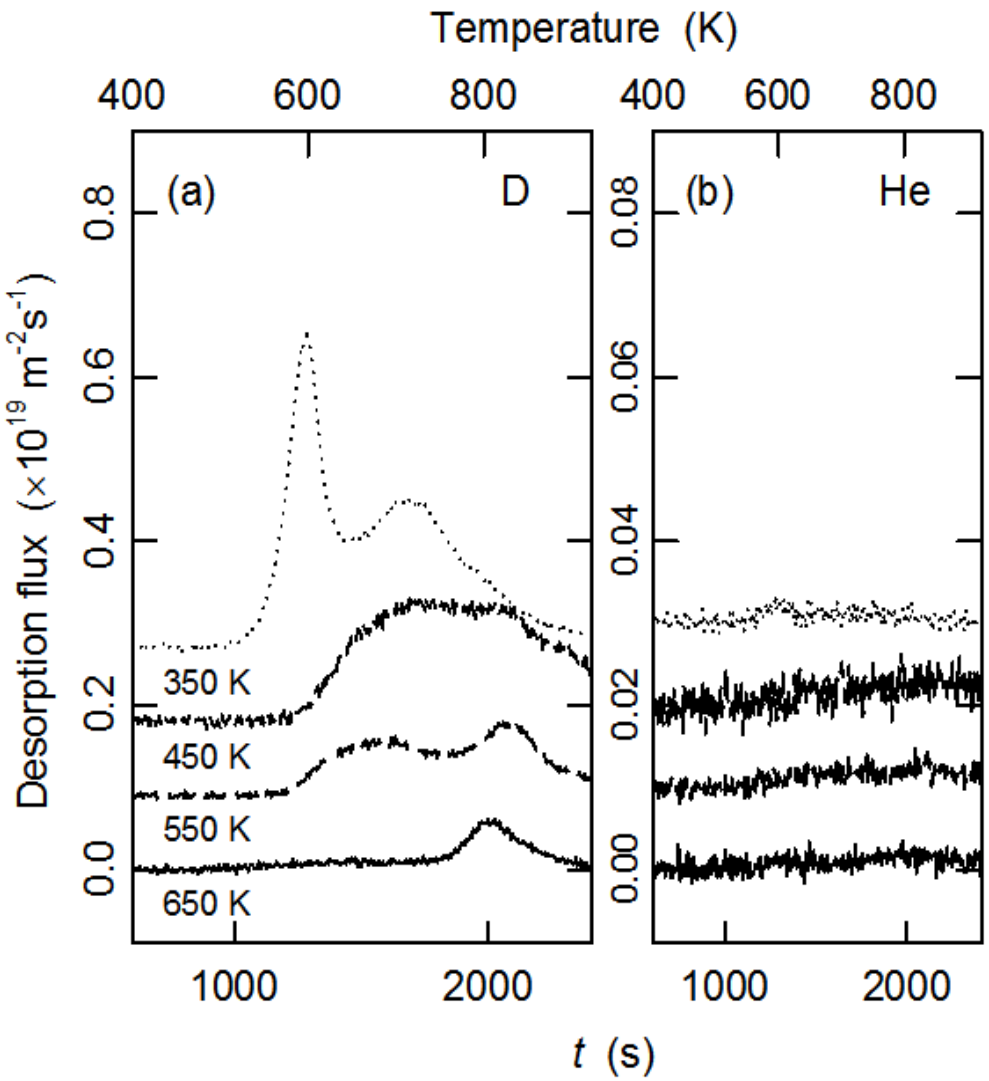


Similar D retention reduction observed in Be

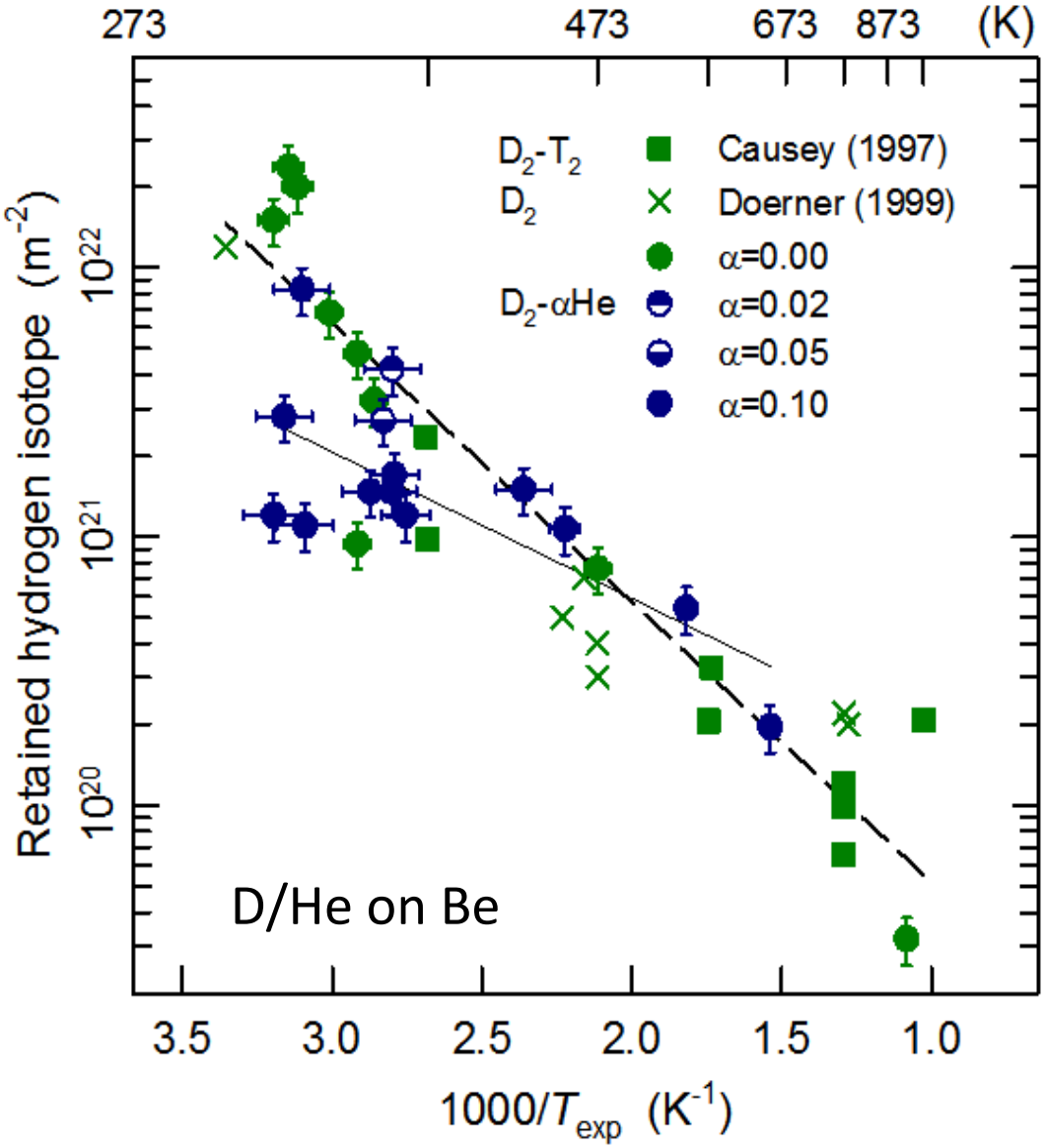
- Vary Sample Temperature During Plasma Exposure
- TDS Emission Spectra
- Results show largest effect in low energy (550 K) release peak

α	0.1	
T_{exp}	**330 – 650**	**(K)**
Φ	5×10^{25}	(m^{-2})
E_i	40	(eV)

Ion Energy, Plasma Fluence Have also been examined



He reduces D retention in Be for <200 C exposure temperatures



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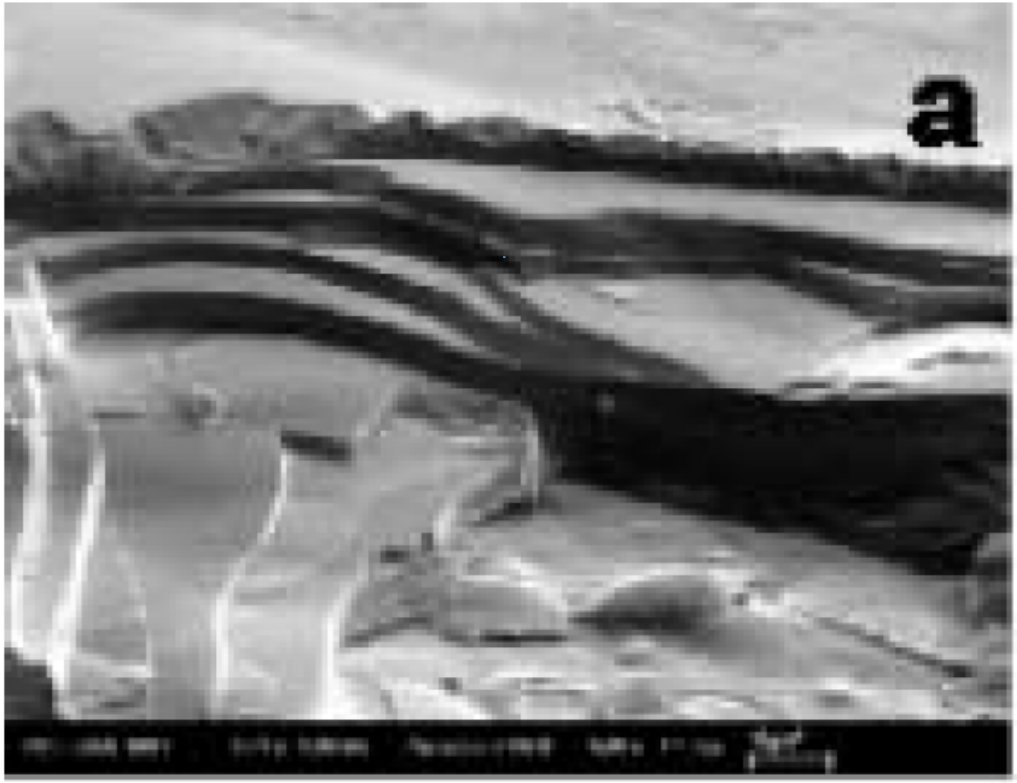
How is the ITER bake efficiency affected by underlying previously baked layers?

- ITER proposes wall/divertor bakes to control T inventory.
  Define as – under layers
- Post bake ITER shots will create new, saturated Be-D/T codeposit layers.
  Defined as – over layers
- Under layers could be fully/ partially desorbed of D/T inventory.
- Does D/T diffuse and re-trap in previously depleted underlayer trap sites?



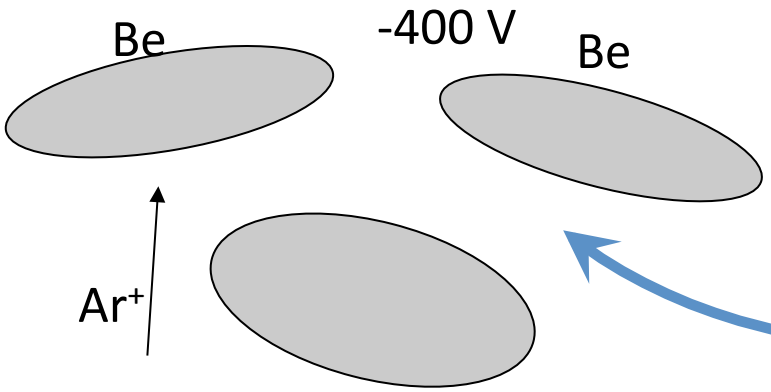
Multi-layered co-deposit in TEXTOR, M. Rubel et al., Phys. Scr. T103(2003)20.

ITER bake studies

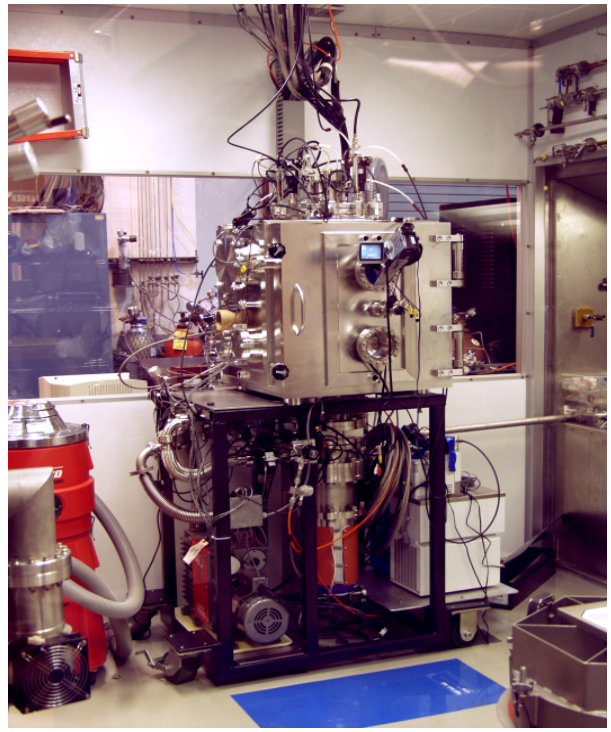
Experiment - details

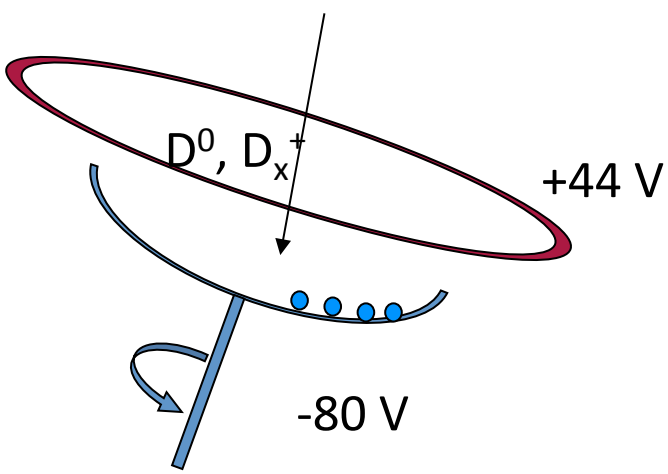
PISCES

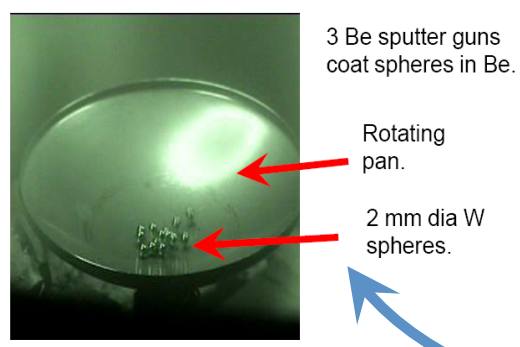
Magnetron sputtering device used to make thick co-deposits, creates batches of identical co-deposits



Utilizes 3, 100 W Be sputter guns/ targets.

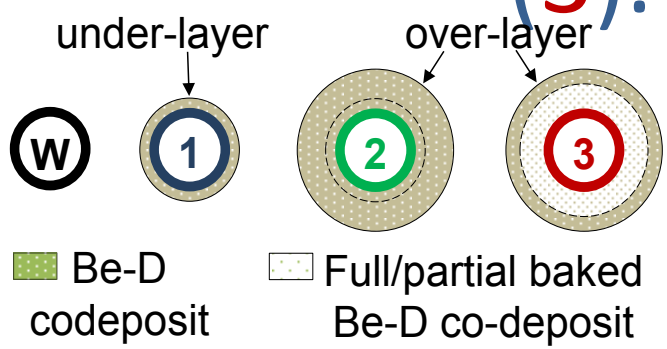






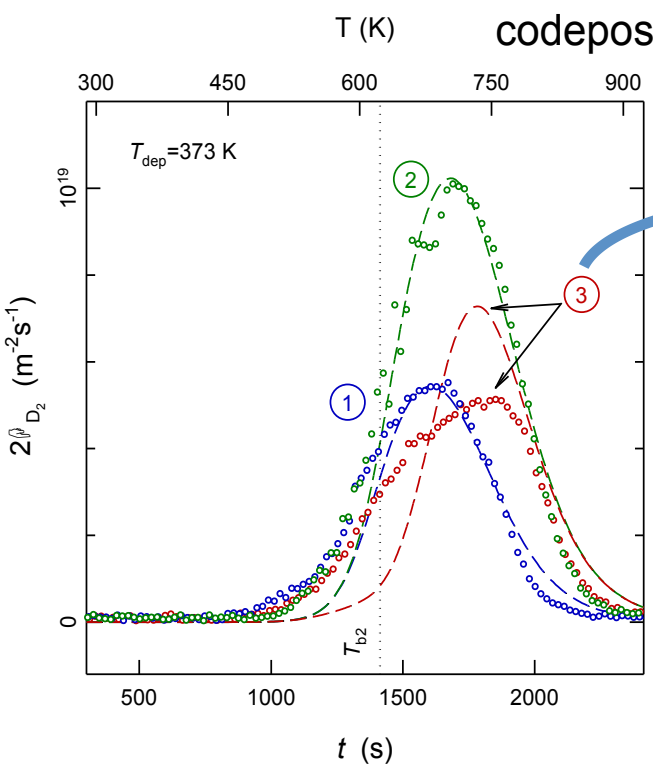
Be-D co-deposited layers 0.2 – 1 µm, thick are deposited on W spheres

TDS & TMAP D release agree well for codeposit thickness (1, 2) variation, but not bake case (3).

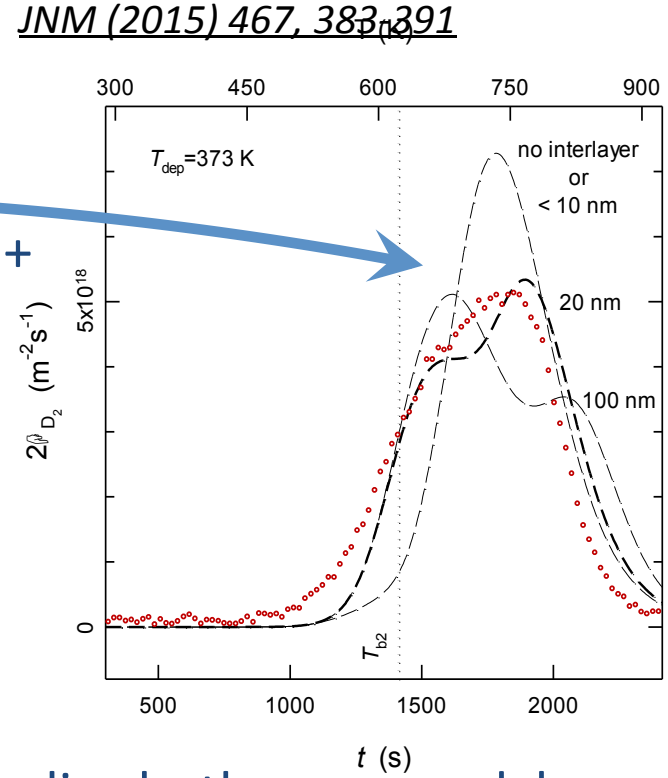


M Baldwin & R Doerner, NF (2014) 54, 083032

M Baldwin & RP Doerner JNM (2015) 467, 383-391



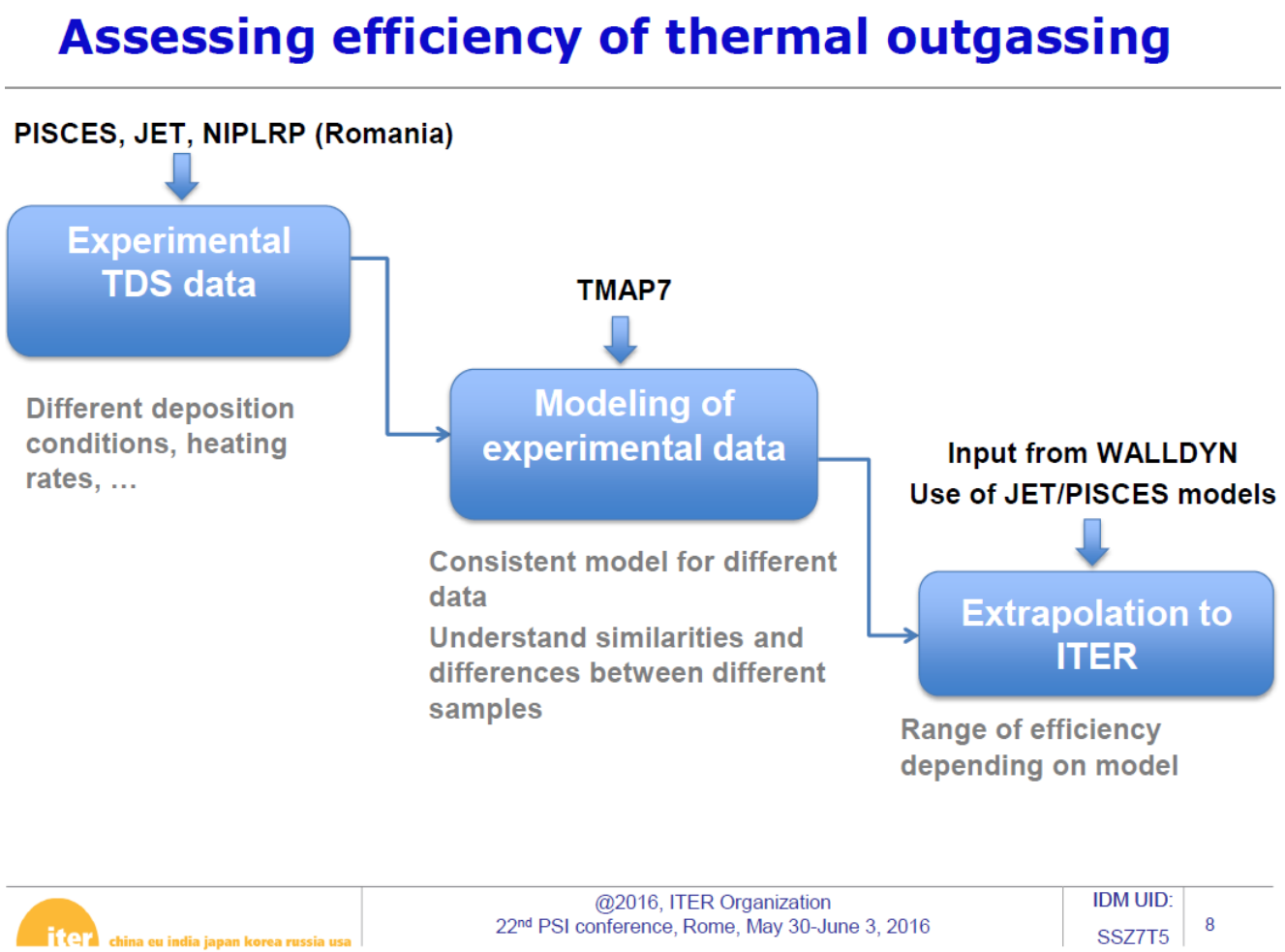
Baked underlayer + new overlayer desorption 3, suggests diffusion barrier interlayer effects.



Surface BeO forms during bake

Implies both more, and less, difficult to remove inventory components.

PISCES TMAP model validation used to evaluate ITER bake strategy



G De Temmerman (ITER) – presented at the 22nd Int. Conf. on PSI, ROME, 2016

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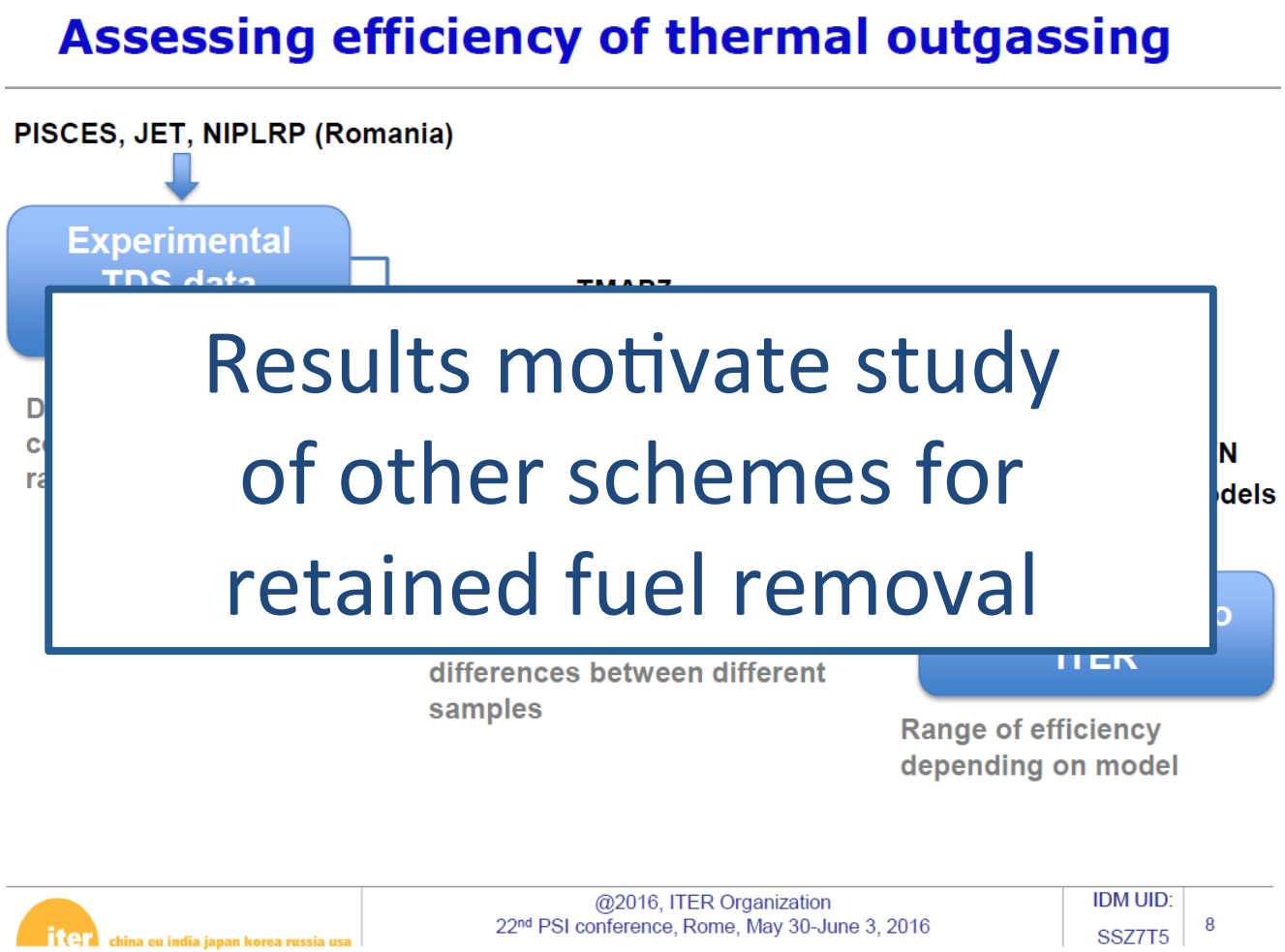

Results motivate study of other schemes for retained fuel removal

G De Temmerman, ITER – presented at the 22nd Int. Conf. on PSI, ROME, 2016

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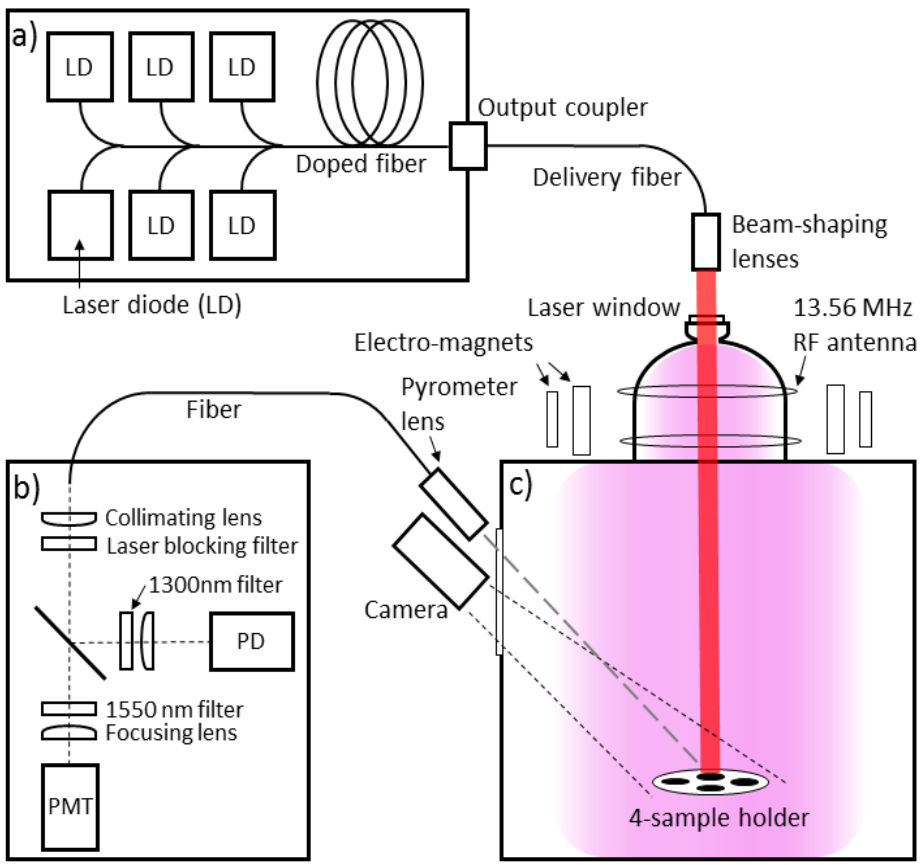
Laser induced thermal desorption experiments: Plasma, laser, and TDS are modeled self-consistently using same model parameters

Plasma → Non-ablative **Laser** (plasma off) → **TDS**

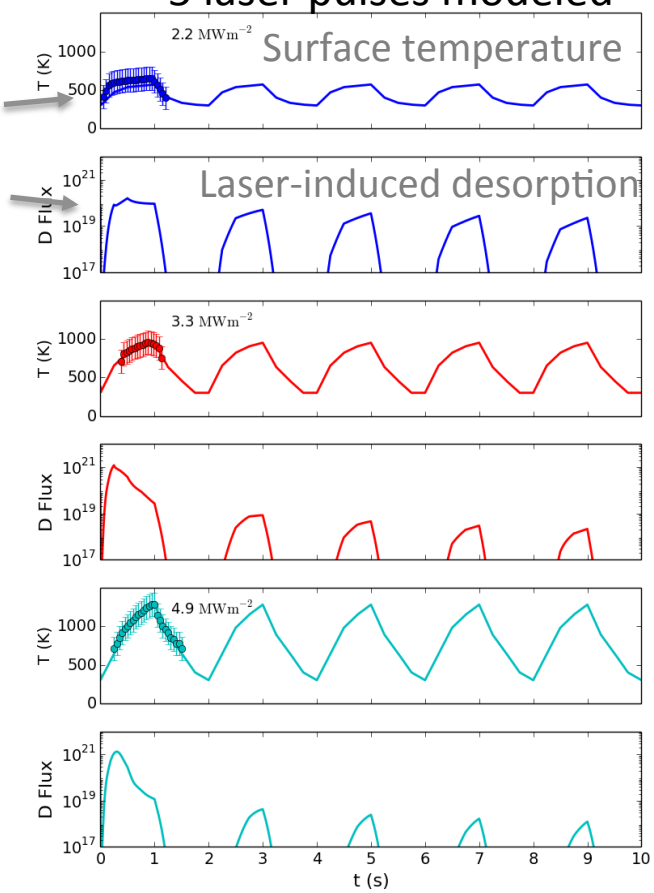
Reference sample



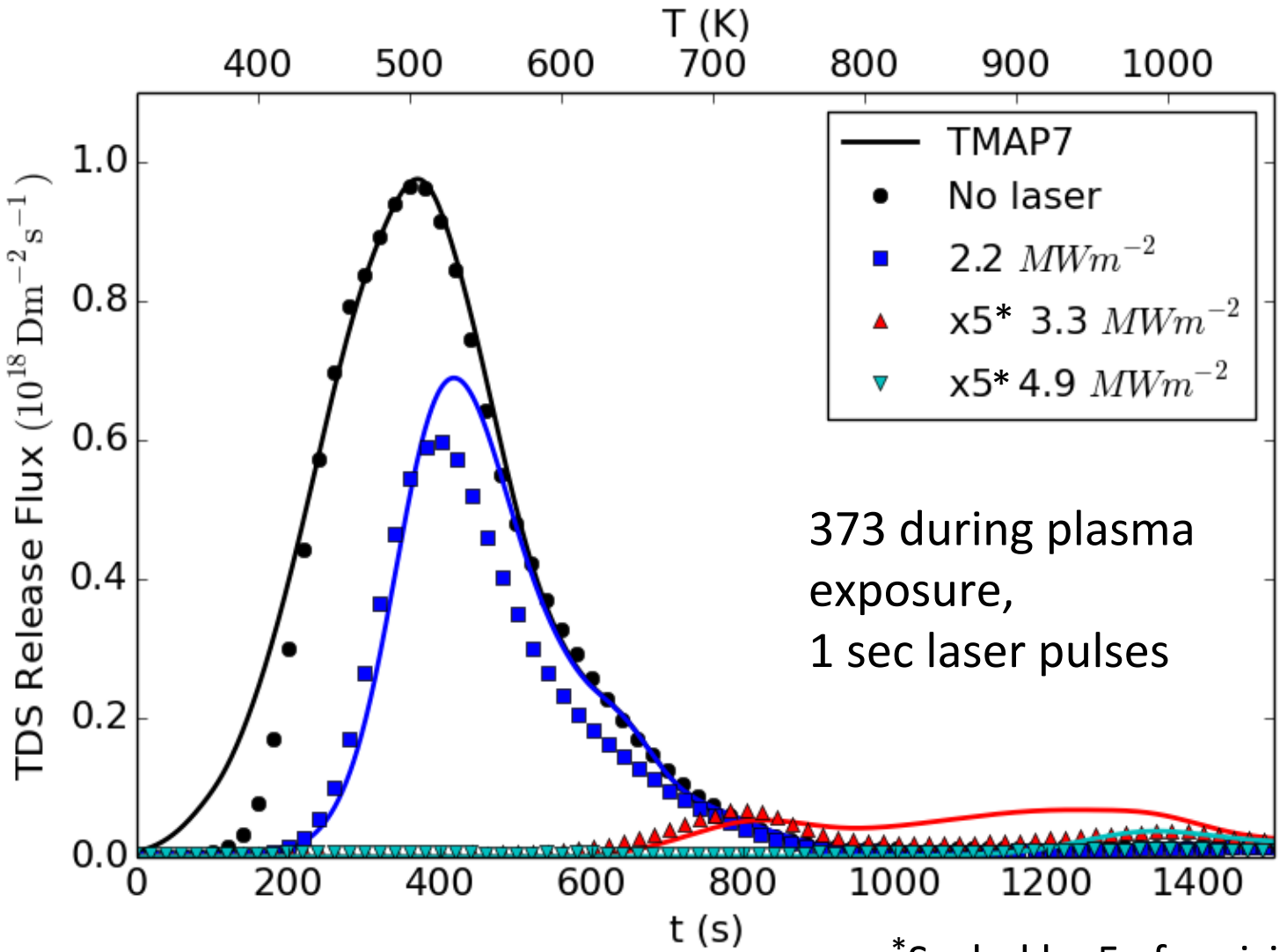
5 laser pulses modeled

Pyrometer used as input to TMAP

TMAP simulation



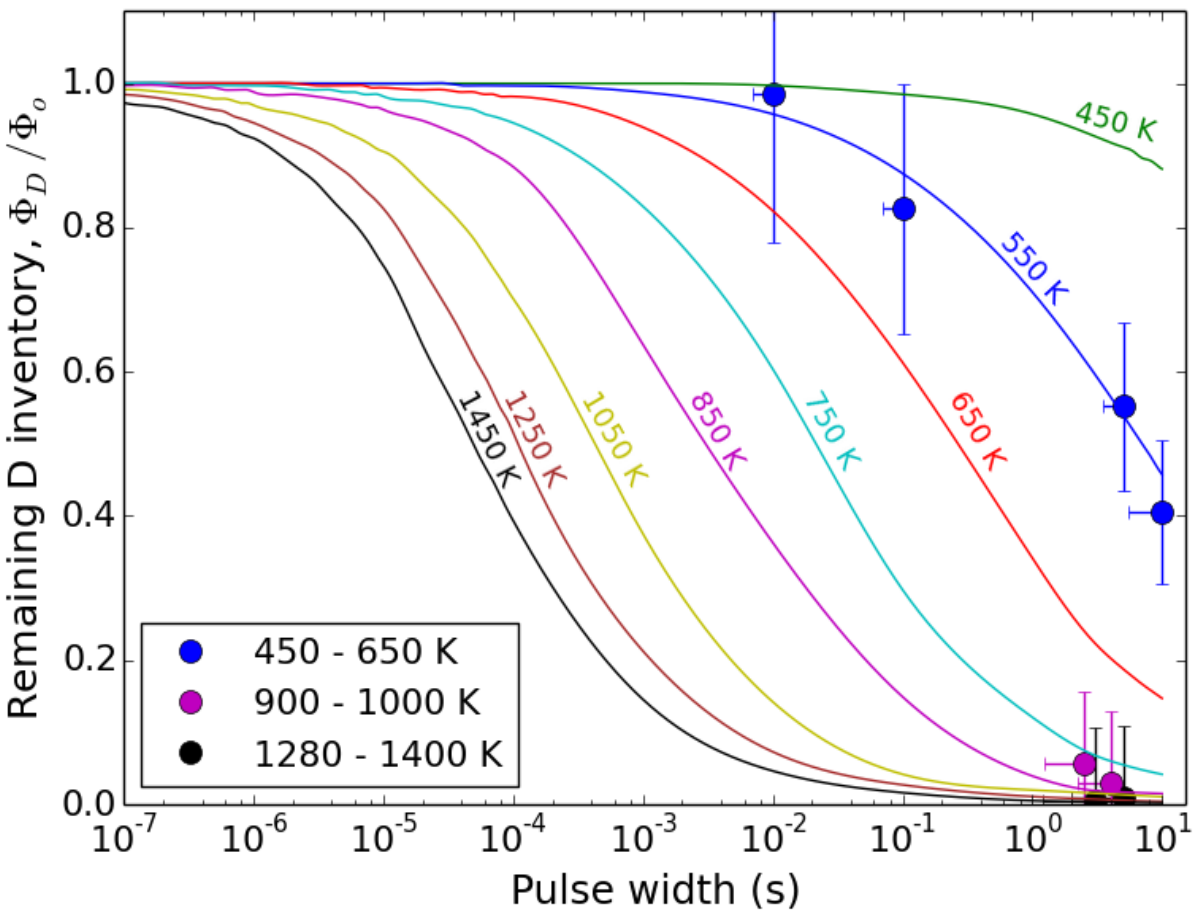
TDS measures remaining D in W after transient laser heating



*Scaled by 5x for visibility

Validated model predicts effective desorption is possible

373 K plasma exposure, $2x10^{20}$ D/(m^2-s)

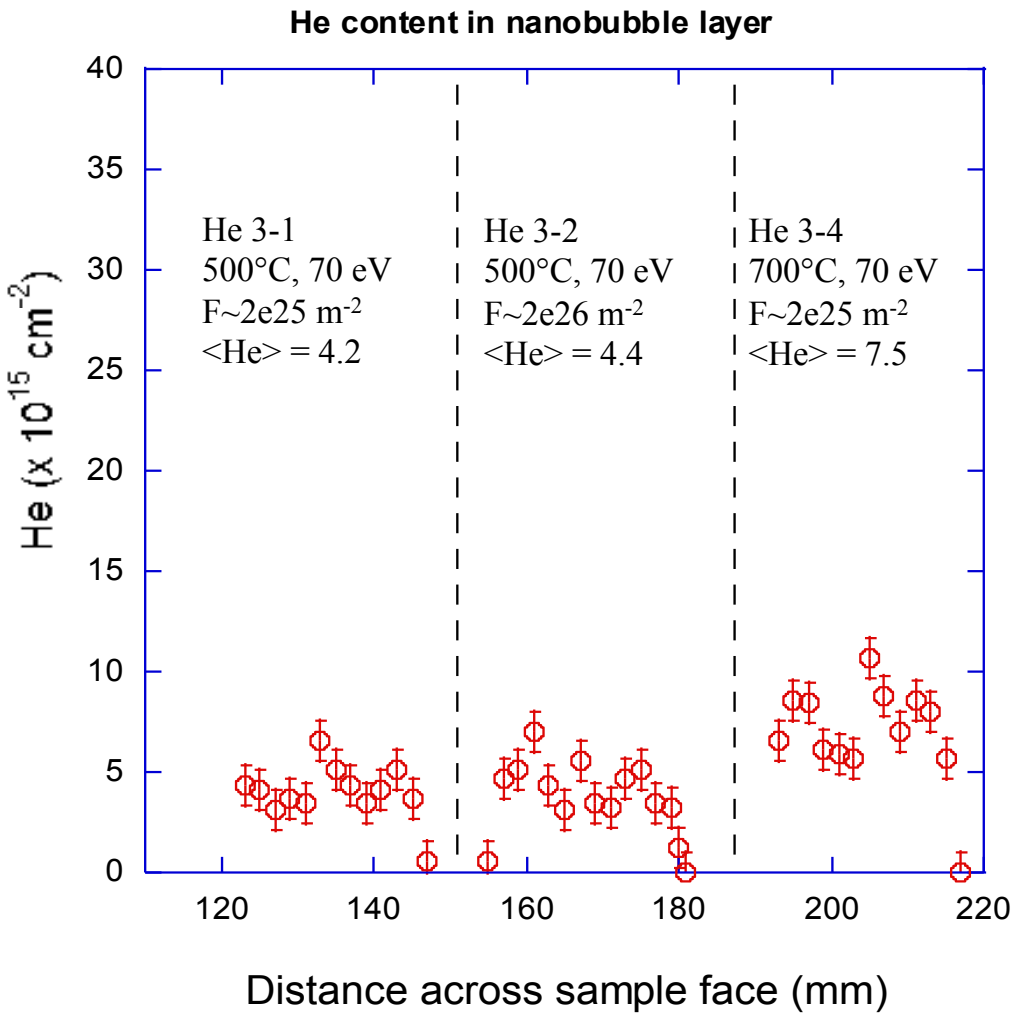


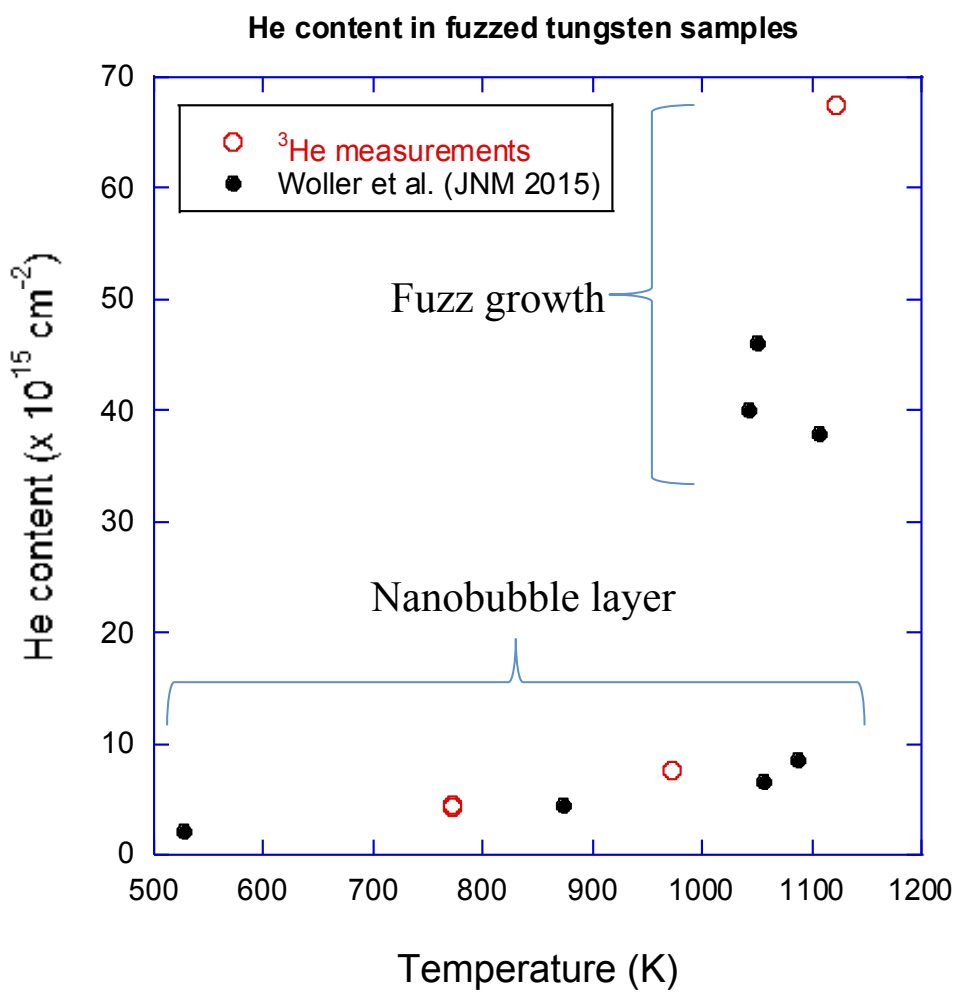
- At T_{peak} = 1280 K for 1 sec pulses, D retention falls below TDS noise floor.
- In addition to T_{peak}, the fraction of desorbed D depends strongly on heating duration.
- Future work: higher sample T needed during plasma exposure for ITER relevance, **but initial results show that thermal detritiation from W is possible.**

He^3 PISCES-A Discharges Permit Measurement of Absolute Concentration of He in Nanobubble Layer

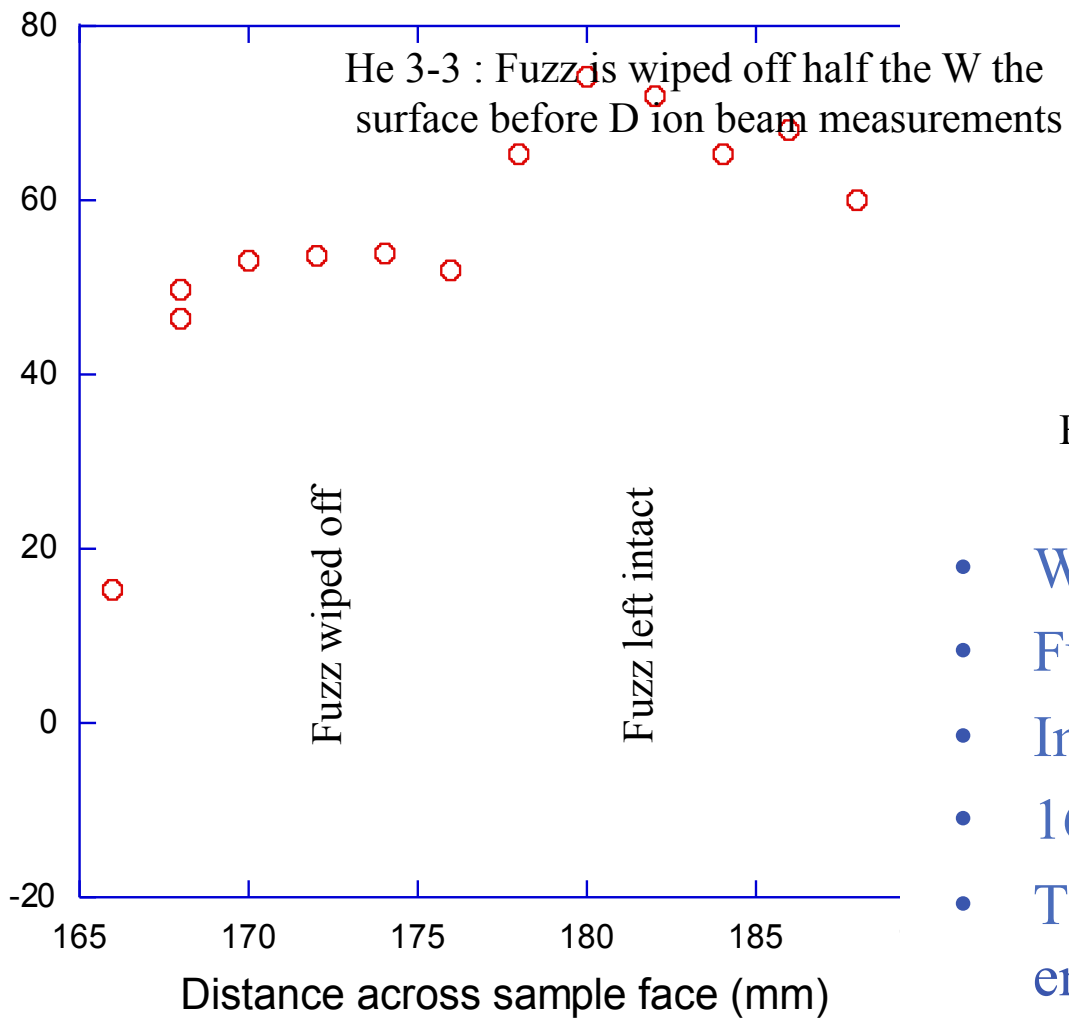
- PISCES-A operation has been modified to allow low gas throughput plasma generation➔ allows ^{3}He plasma generation
- Woller et al. (JNM 438(2013)S913 & JNM 463(2015)289) measured 1-7 at% He in W below, within, and above the W-fuzz formation temperature, <u>with no loss of He after termination of the plasma exposure</u>
- NRA using a D ion beam can then be used to quantify the amount of ^{3}He after plasma exposure using the ^{3}He(D,^{4}He)p nuclear reactions

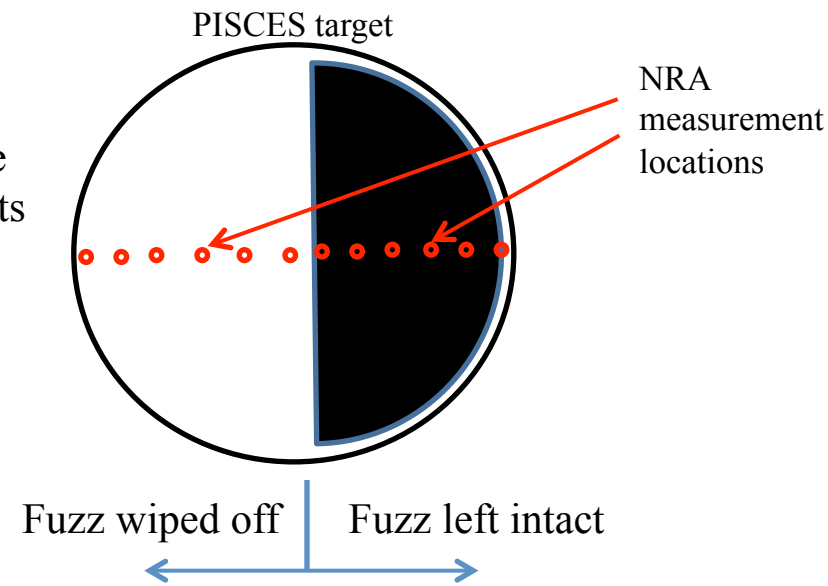
He content in nanobubble layer saturates with fluence, increases slightly with temperature until fuzz forms





Most He resides in the 'growth plate' between the bulk and the fuzz





- W mass loss = 96e-6 g
- Fuzz thickness ~1.5 microns
- Implies ~98% porosity
- 16.4e15 He/cm^{-2} missing
- Therefore, He/W averaged over entire length of tendril ~ 10 at.%

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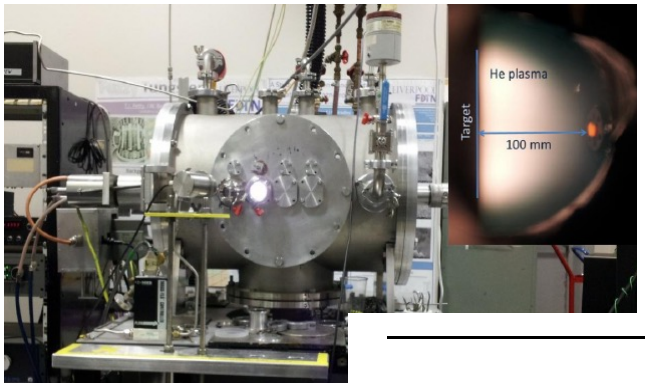
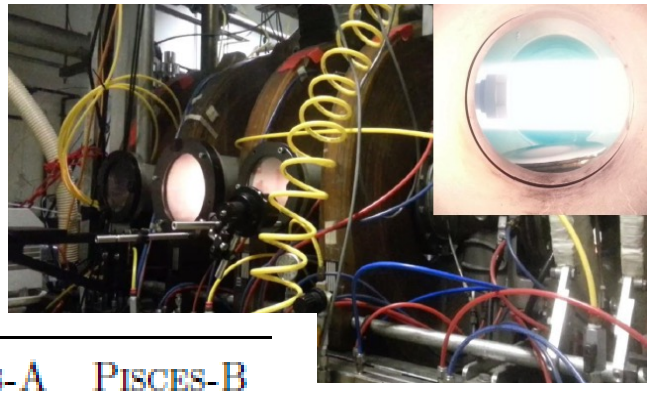
W fuzz growth: He^+ flux dependence explored

PISCES



- W exposed to 4 orders of He plasma ion fluence at 1120 K.



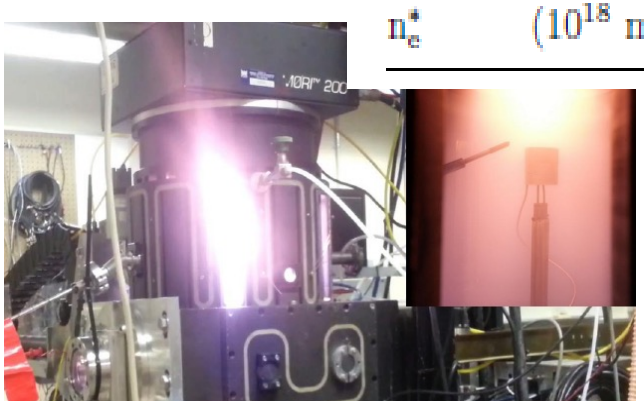
UoL
(Magnetron)

PISCES-E
(Low *p*, R.f.)

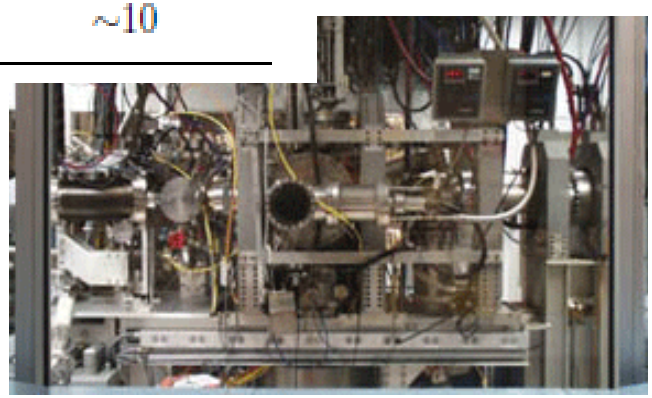
PISCES-A
(reflex arc)

PISCES-B
(reflex arc)

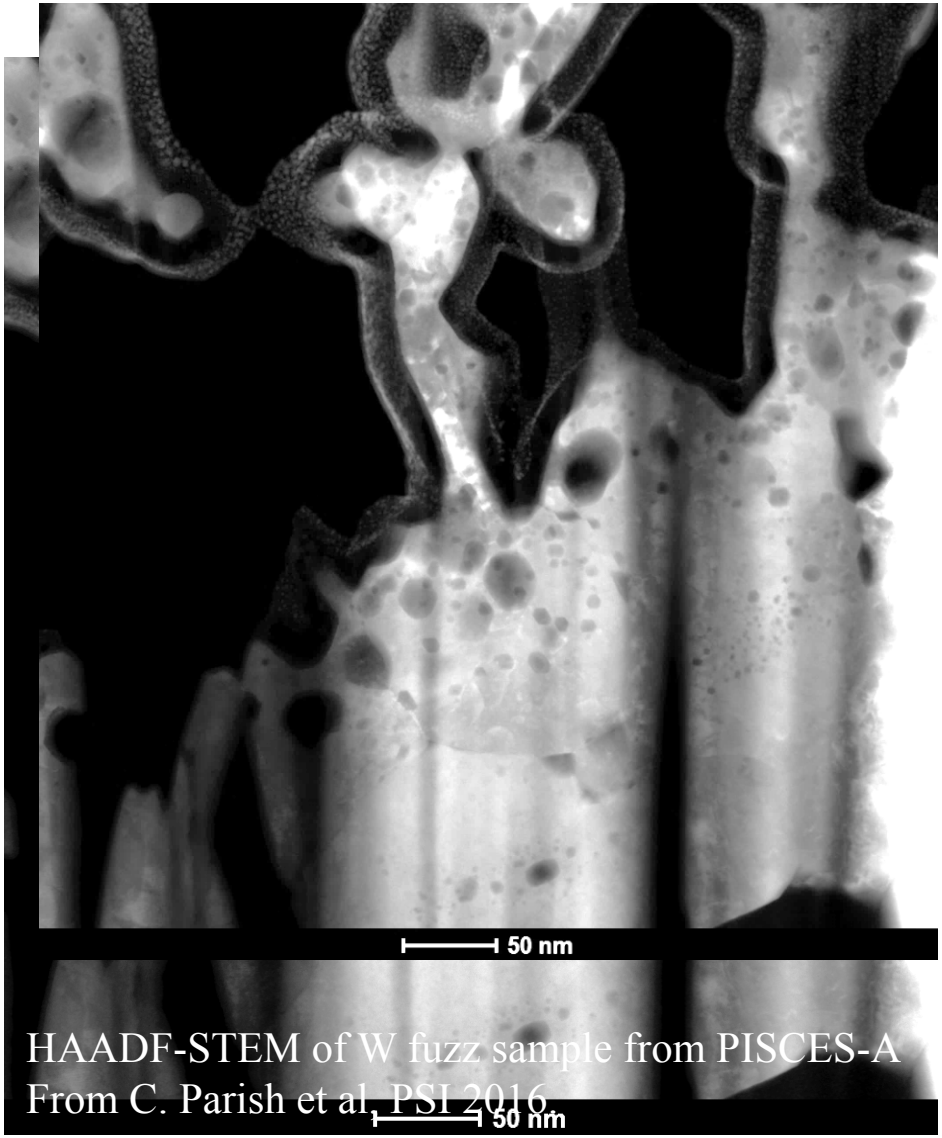
		UoL Mag.	PISCES-E RF	PISCES-A DC arc	PISCES-B DC arc
$P^*_{disch.}$	(kW)	0.7	1.3	1.5	3.0
Γ	(10^{22} $m^{-2}s^{-1}$)	0.001-0.01	0.01-0.5	0.5-8	5-20
$\Phi^\dagger$	(10^{26} m^{-2})	0.01-0.1	0.1-5	5-80	50-200
T^*_e	(eV)	~7	~4	~6	~6
n^*_e	(10^{18} m^{-3})	~0.01	~0.5	~5	~10



- 4 plasma devices utilized
- $t^{0.5}$ growth rate further explored.



A bubble-rich layer exists between the W bulk and the W fuzz ➔ suggests roll for bubbles in fuzz growth



HAADF-STEM of W fuzz sample from PISCES-A
From C. Parish et al, PSI 2016

From S. Kajita et al, JNM 418(2011)152

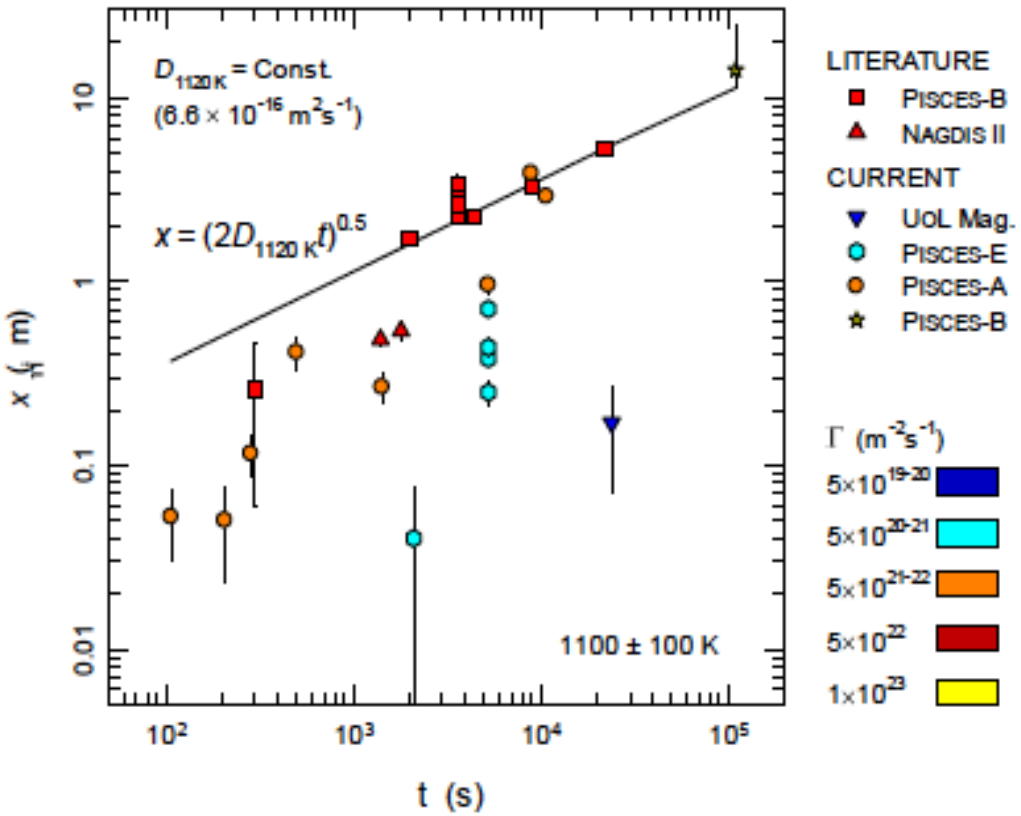
Fuzz layer thickness x, $\propto$ to fluence, $\Phi^{0.5}$. ($t^{0.5}$ for const. ion flux)

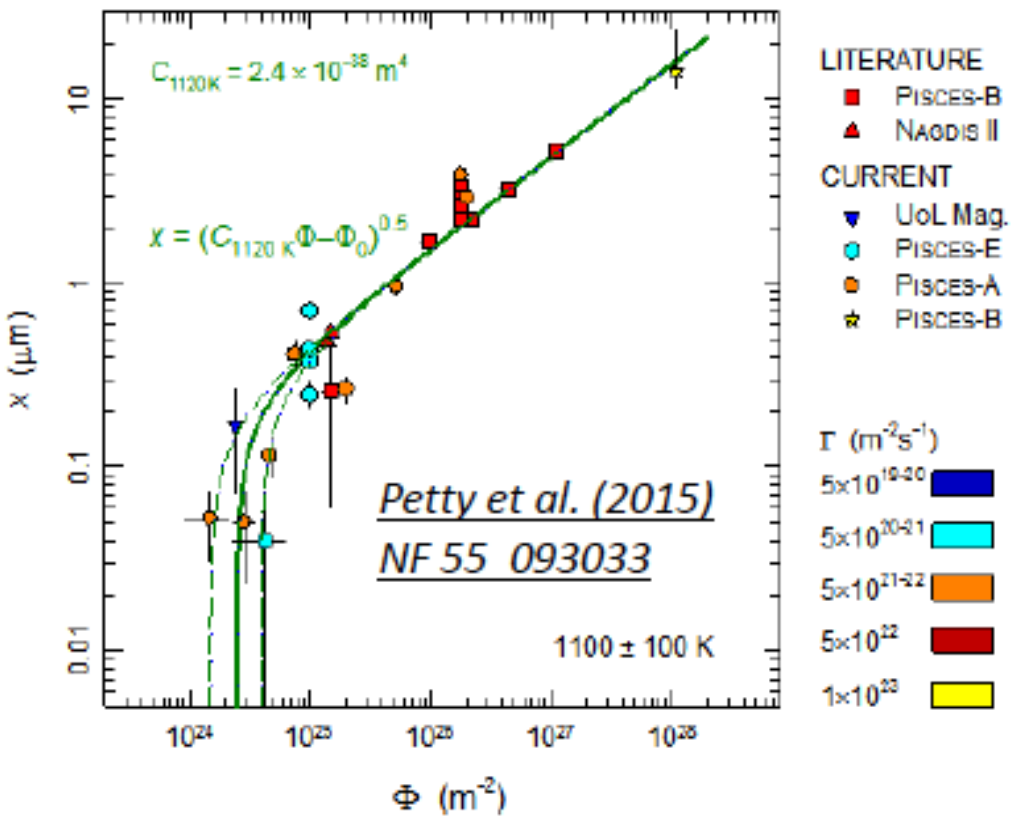
$t^{0.5}$, in lower He ion flux regimes does not give consistent layer growth with PISCES-B.

Re-examination further suggests the necessity of an incubation He fluence, Φ_0, prior to fuzz growth

Problem is re-examined.

$$x(\Phi) = (C(\Phi - \Phi_0))^{0.5}$$





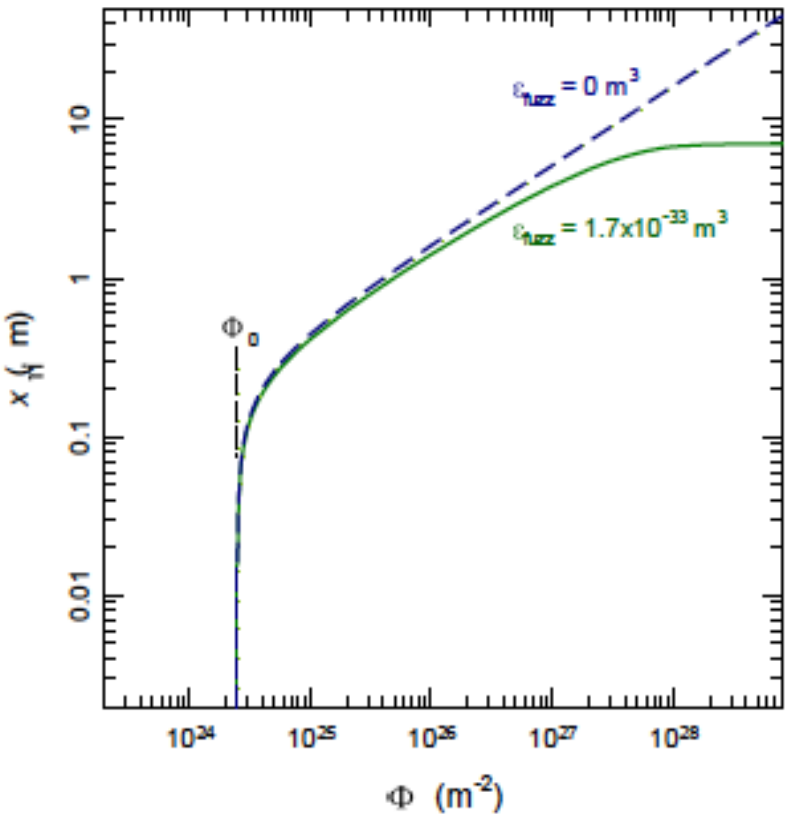
Fuzz growth-erosion problem re-examined in light of fluence dependence

$$dx/d\Phi = C/2x - \epsilon_{\text{fuzz}}$$

where ϵ_{fuzz}: fuzz erosion velocity, normalized to flux - units in [m^3].

$$\epsilon_{\text{fuzz}} \cong \kappa\frac{(1-p)}{(1-p)}Y_{\text{bulk}} \qquad \epsilon_{\text{fuzz}} \cong \kappa\frac{1}{(1-p)}Y_{\text{fuzz}}$$

where $\kappa = \mathrm{m_W}/\rho_{\mathrm{W}}$: $\mathrm{m_W}$: tungsten at. mass and, ρ_{W}: W density, p: porosity



No Erosion Case: ($\varepsilon = 0$)

$$x(\Phi) = (C(\Phi - \Phi_0))^{0.5}$$

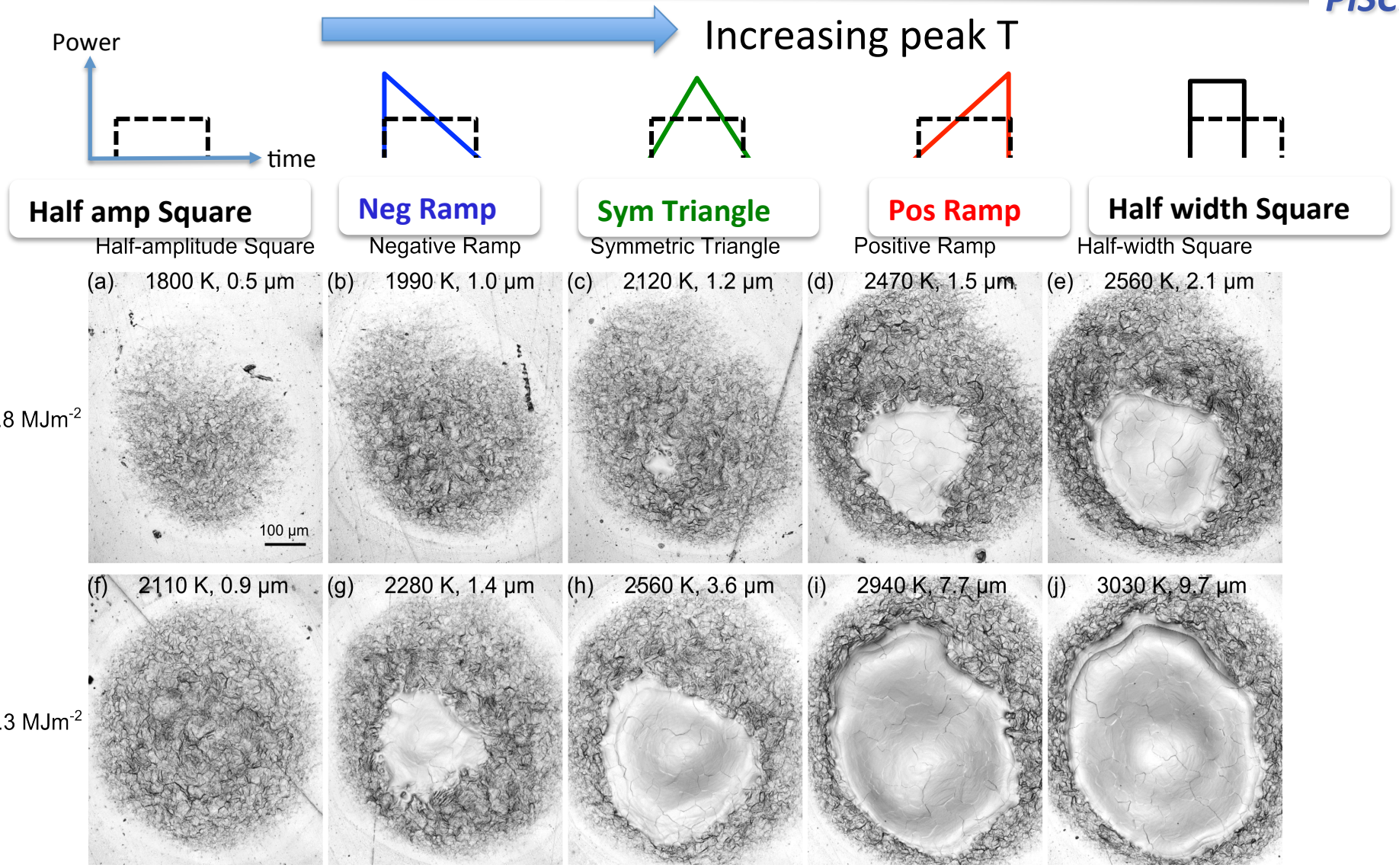
Erosion Case: ($\varepsilon > 0$) (Lambert **W** function)

$$x(\Phi) = \frac{C}{2\epsilon_{\text{fuzz}}}\left(\mathbf{W}\left[-\exp\left(\frac{-2\epsilon_{\text{fuzz}}^2}{C}(\Phi - \Phi_0) - 1\right)\right] + 1\right)$$

PISCES Supporting ITER PMI Needs

- Record Fluence Exposures Show No Saturation of D Retention in W
- He nanobubble formation inhibits D retention in W; similar results observed in Be
- Progress on identifying mechanism of D retention suppressi
- ITER bake studies guide plans for T inventory control
- Discovered workable alternate T inventory control techniqu
- Successful modeling of W-fuzz formation
- **Controlled ELM-like thermal transients more clearly define damage thresholds for W divertor target**

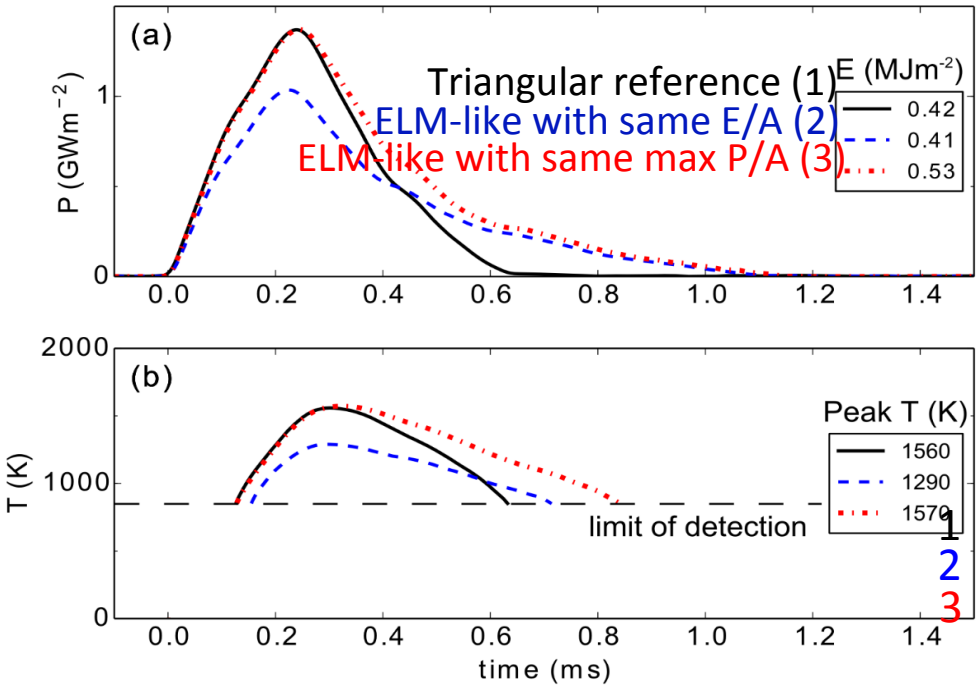
Transient heating damage depends on pulse shape



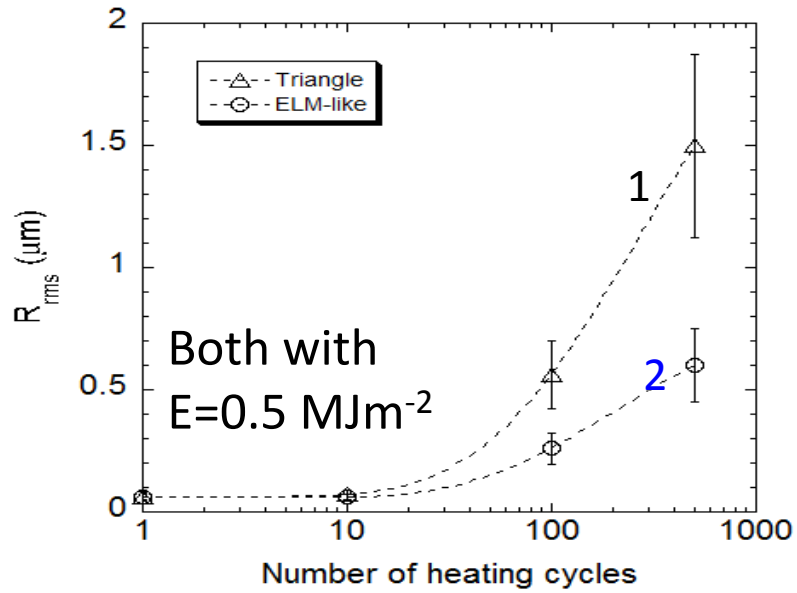
For a given energy density and peak power, a square pulse creates the highest peak surface T

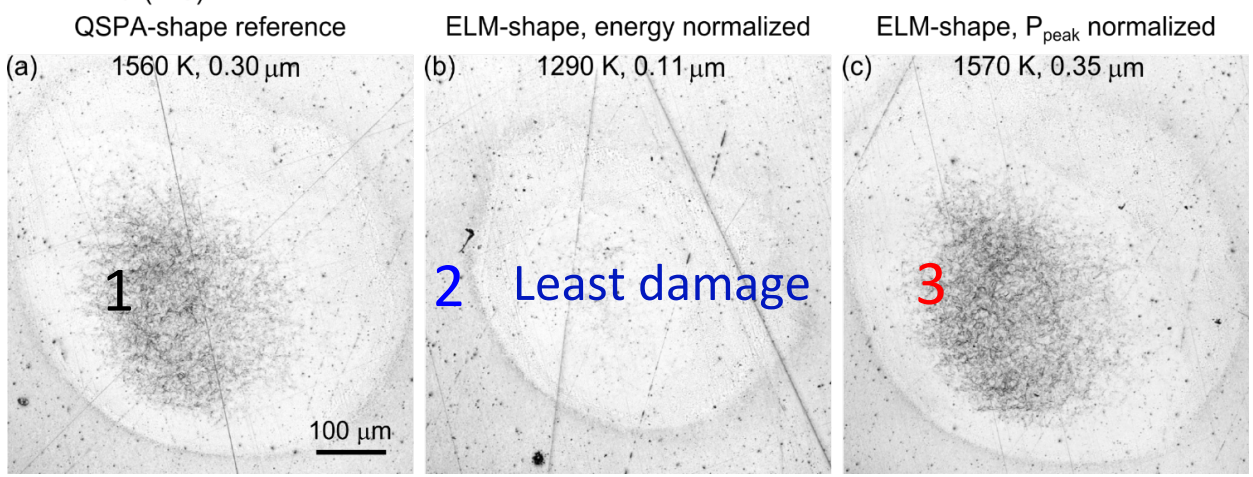
ELM-shaped pulses show less damage than triangular shapes used to establish the ITER ELM damage threshold

PISCES



Surface roughness vs. number of pulses





N=100

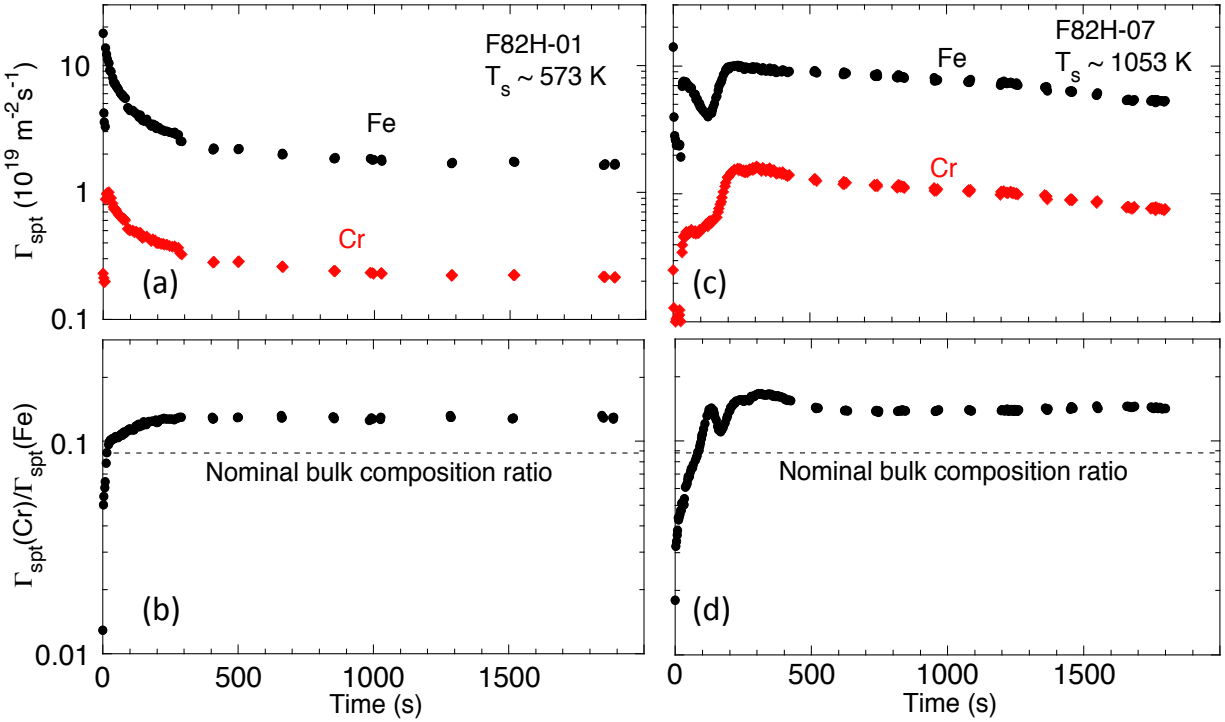
PISCES Supporting Fusion Nuclear Science

- **RAFM Steel Erosion Studies (w/ IPP-Garching)**
- Plasma & displacement damage effects on PFC thermo-mechanical properties
- Displacement damage effects on D Retention & Removal (UC-funded collaboration w/ LANL)
- Simultaneous displacement damage/He production effects on D Retention
- Divertor Physics, In-situ PMI Diagnostic Development
- Material Migration Studies

Reduction of the sputtering yield of RAFM steels is observed under high-flux He plasma exposure.

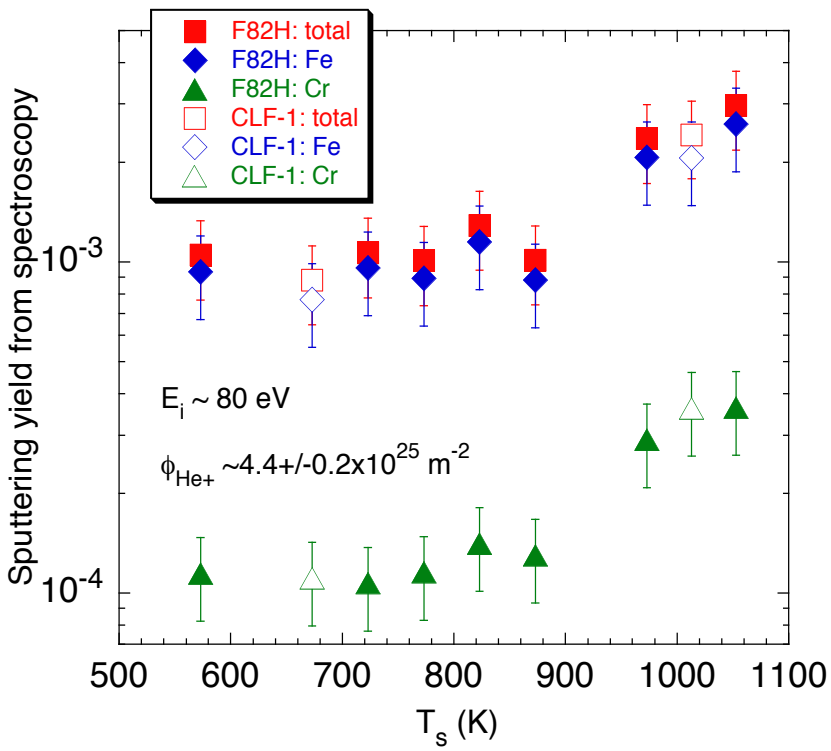
- In future fusion reactors, use of reduced activation ferritic/martensitic (RAFM) steel as a first wall material is considered an attractive option.
- **S/XB values of Fe I and Cr I lines were experimentally determined to quantify the sputtered flux of each species** (Fe, Cr, W). (W I S/XB values were previously measured.)

- No W I lines were observed.
  - **Preferential sputtering of Fe and Cr**.
- The reduction is faster for lower T_s.
  - Slower diffusion of Fe and Cr.
- The sputtered flux ratio, Cr/Fe, is higher than the nominal bulk composition ratio.
  - The diffusion of Cr to the surface is faster than Fe.

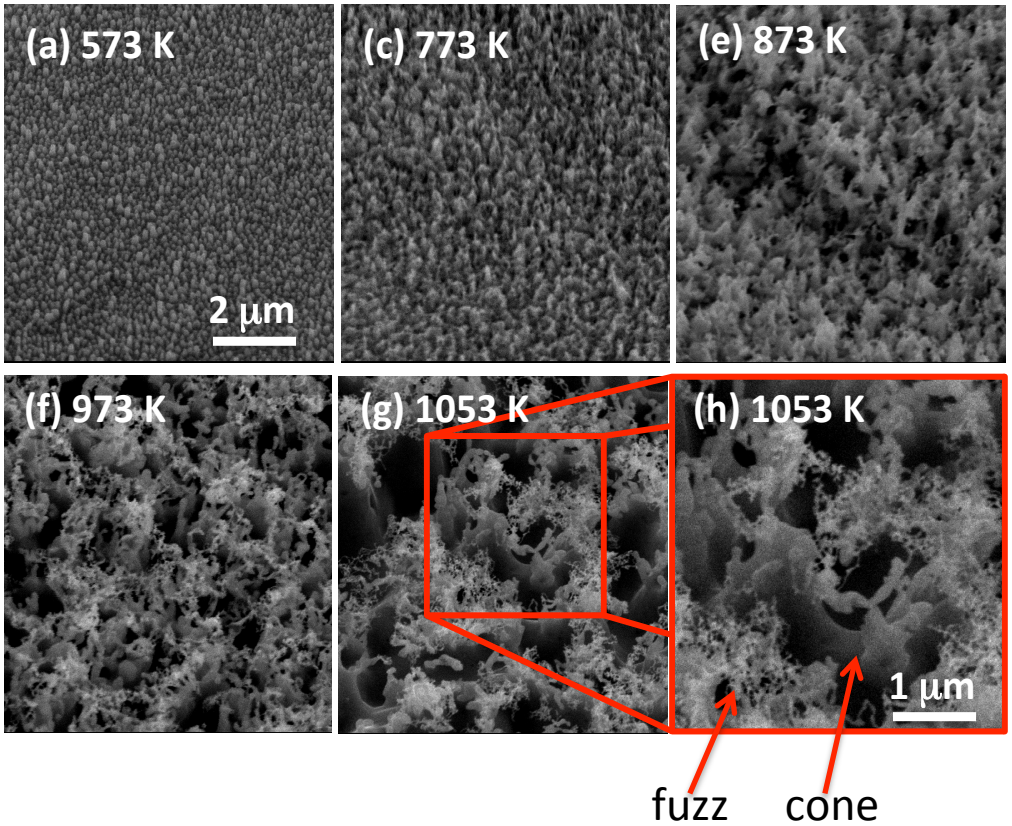


The sputtering yield is found to be constant up to T_s ~ 900 K, and to be enhanced at $T_s \geq 900$ K

- The enhanced erosion is due to **less W coverage** (AES) and **larger sputter cones** (SEM) at $T_s \geq 900$ K.



- Cone-like structures become larger with increasing T_s.
- W fuzz is clearly seen on top of the cones at $T_s \geq 973$ K.



PISCES Supporting Fusion Nuclear Science

- RAFM Steel Erosion Studies (w/ IPP-Garching)
- **Plasma & displacement damage effects on PFC thermo-mechanical properties**
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- Simultaneous displacement damage/He production effects on D Retention
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- Material Migration Studies

Experimental Approach

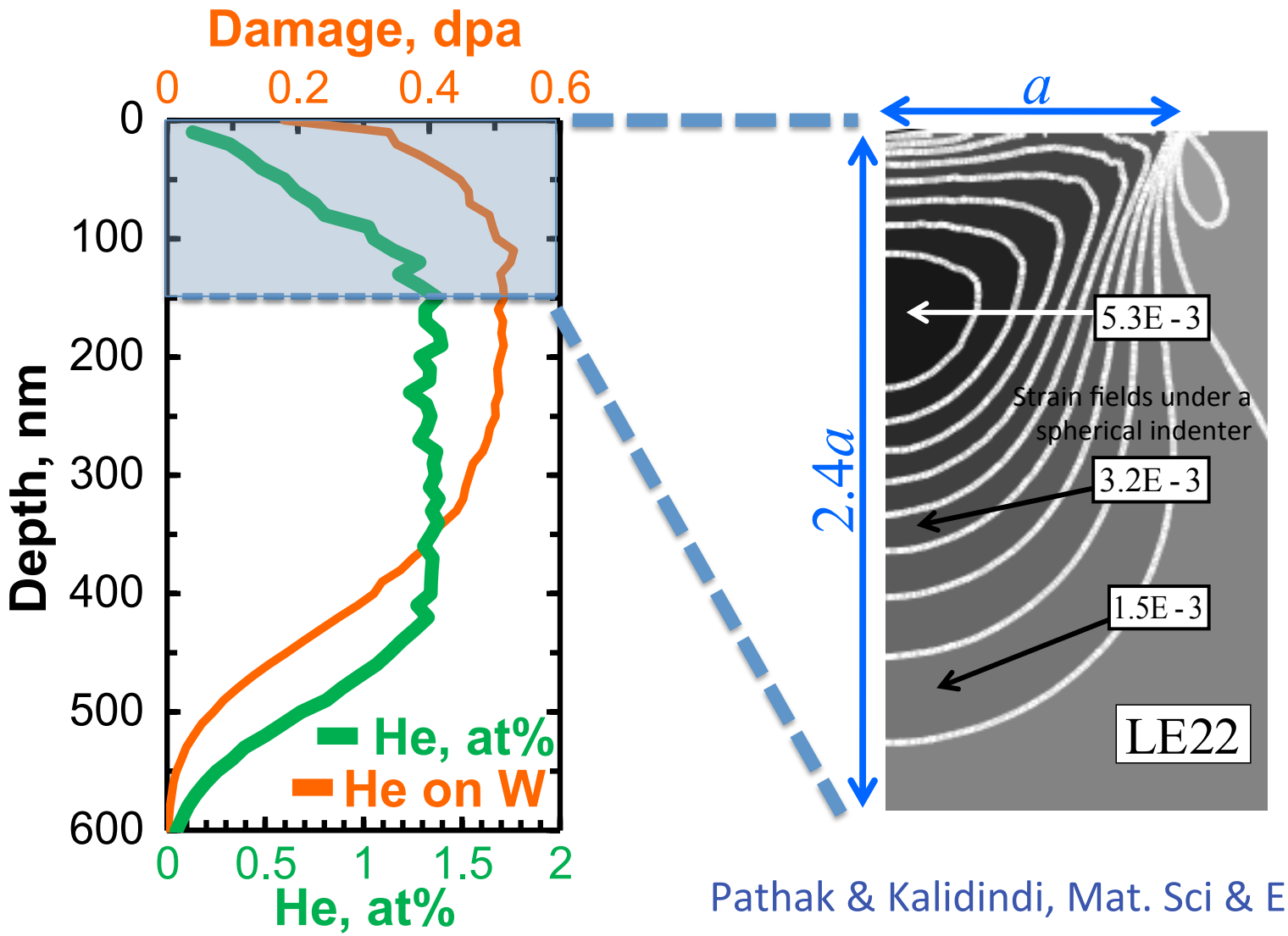
Thermo-mechanical properties:

- Energetic (0.5-5 MeV) He, Cu, W Ion Beams to induce displacement damage;
  - Nanoindentation for Modulus & Hardness of damaged region
  - 3ω thin-film thermal conductivity of damaged region

D Retention:

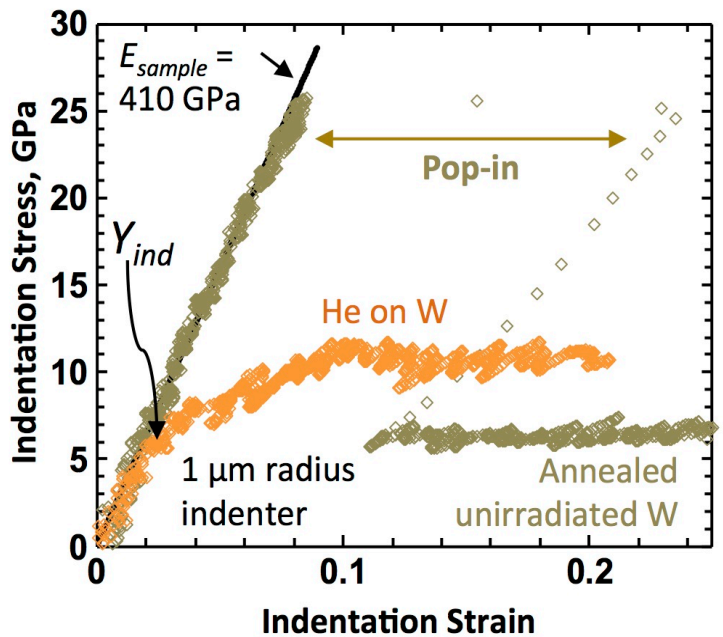
- Control damaging temperature from 300-1200K
- Plasma implanted D at 100eV, low temperature (380 K) to decorate damage sites
- NRA, TDS for retention

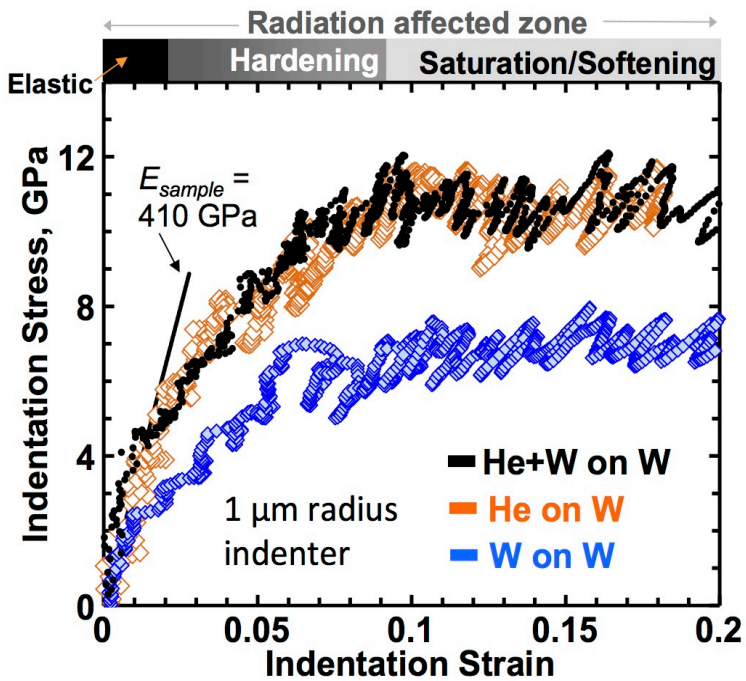
Nano-indentation stress-strain measurements ***localized within*** damaged layer

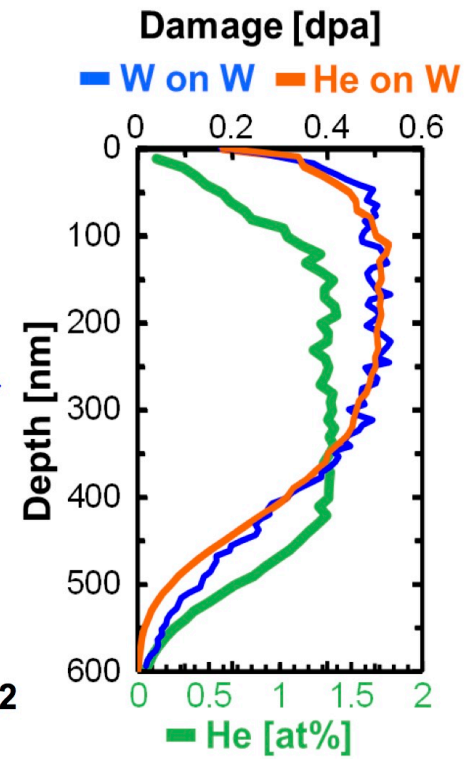


Pathak & Kalidindi, Mat. Sci & Eng R (2015)

Modulus unchanged & increased hardness with 0.5 dpa He, W damage



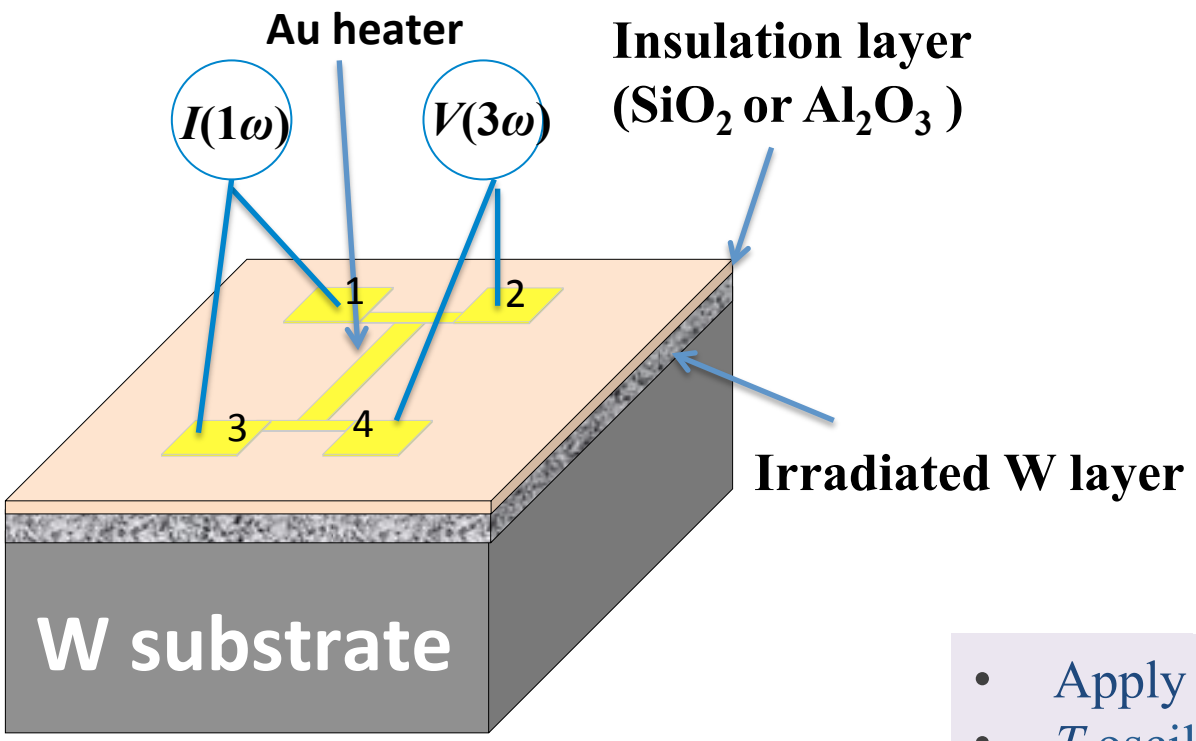


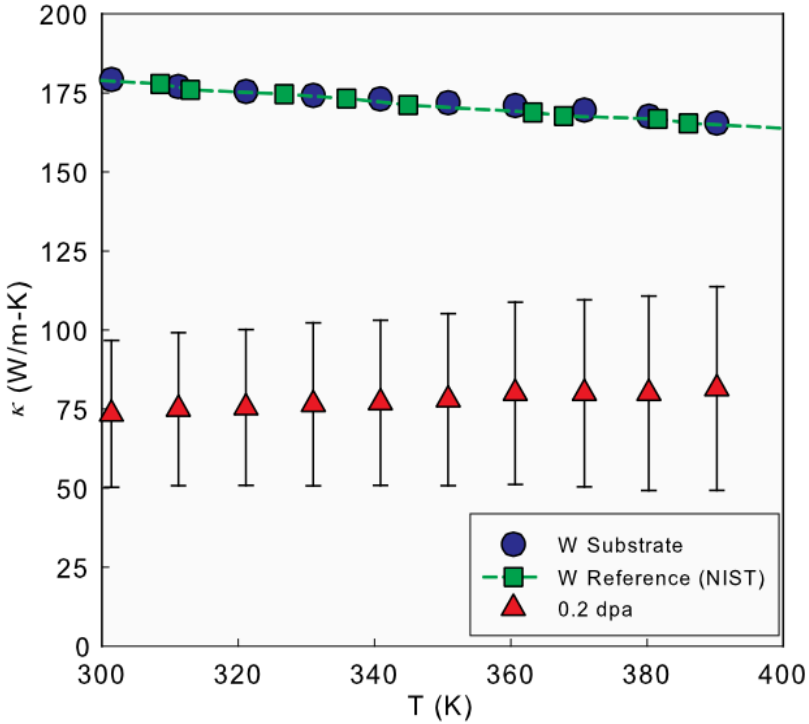


Pathak & Kalidindi, Mat. Sci & Eng R (2015),
Tynan, PSI-'16, submitted '16

Thin-film techniques probe thermal conductivity *localized within* damaged layer

3ω method



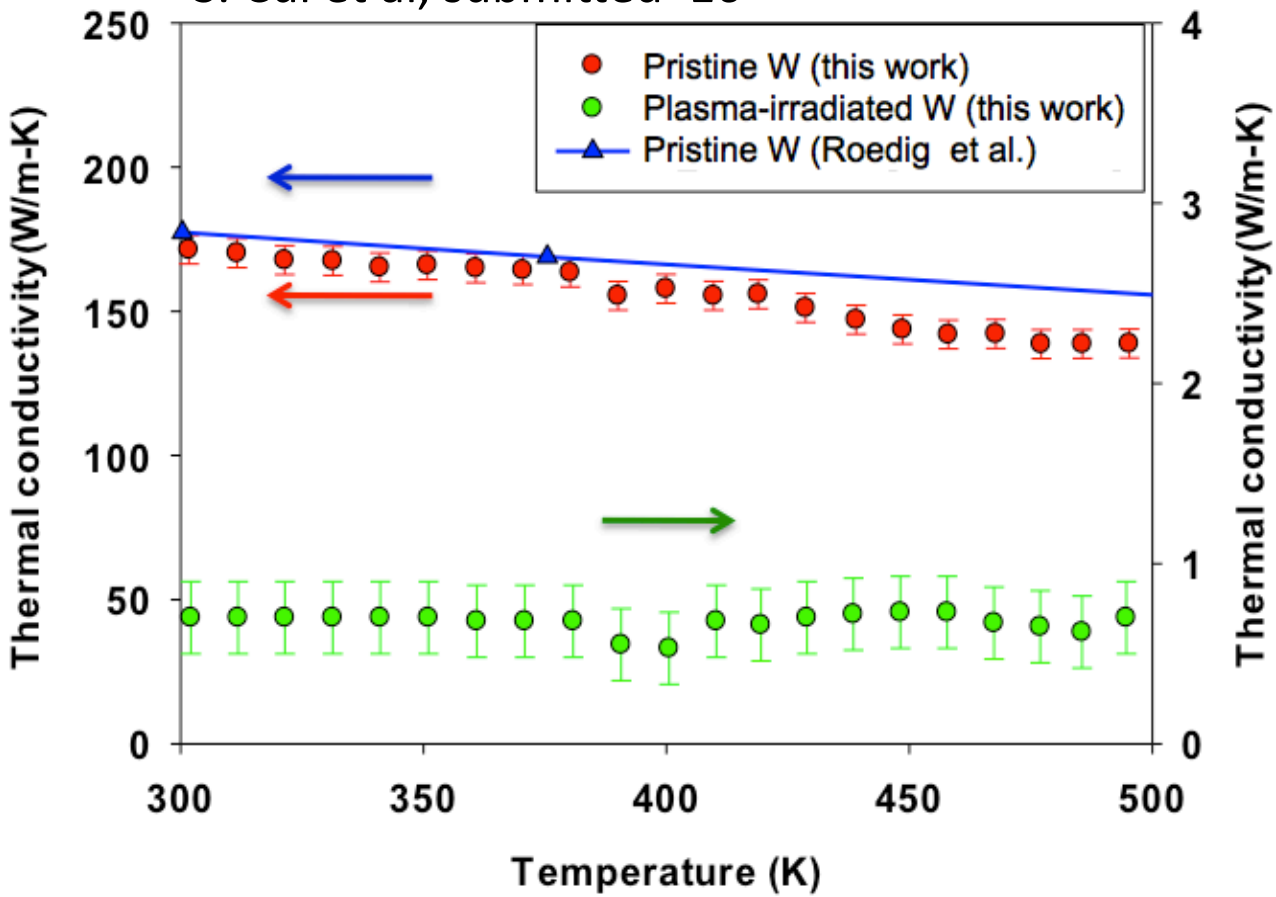


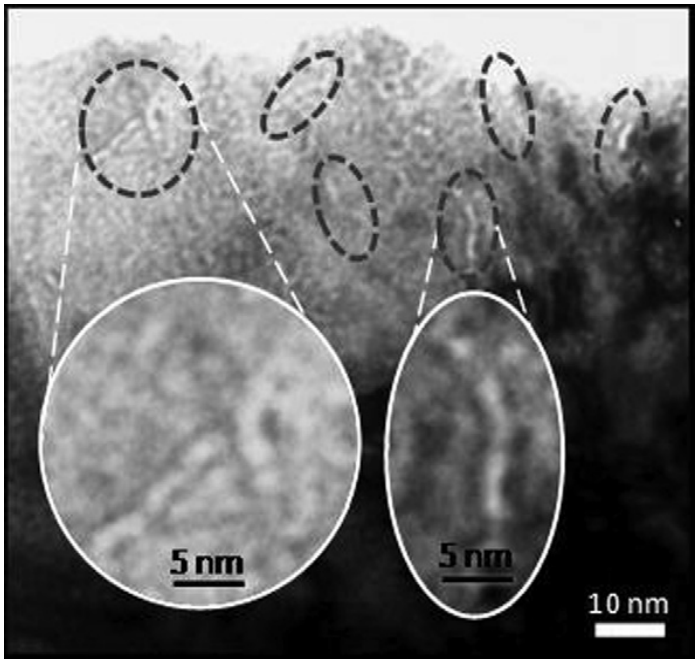
- Apply $I(\omega)$
- T oscillates at 2ω by Joule heating ($Q = I^2R$)
- R oscillates at 2ω ($R=R_o+\alpha T$)
- Can measure T rise from $V(3\omega)$
  - $V_{3\omega} = I(\omega)R(2\omega)$
  - Solve heat transport eqn to infer κ

Dechaumphai *et al.*,
J Nucl. Mater., 455 (2014) 56–60

Large (200x) Reduction in Thermal Conductivity of He nano-bubble layer in W

S. Cui et al, submitted '16

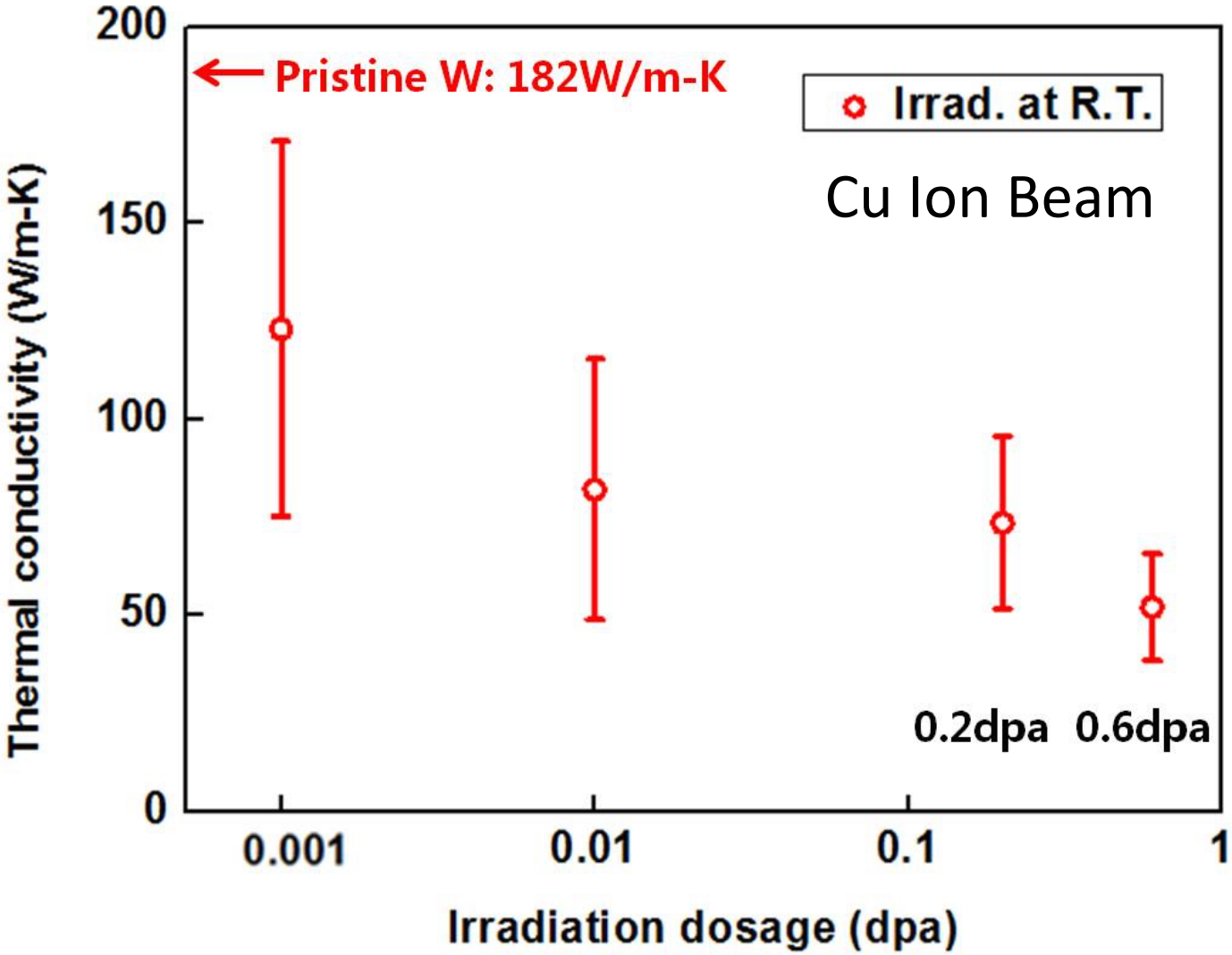




M. Miyamoto et al., JNM 415 (2011) S657

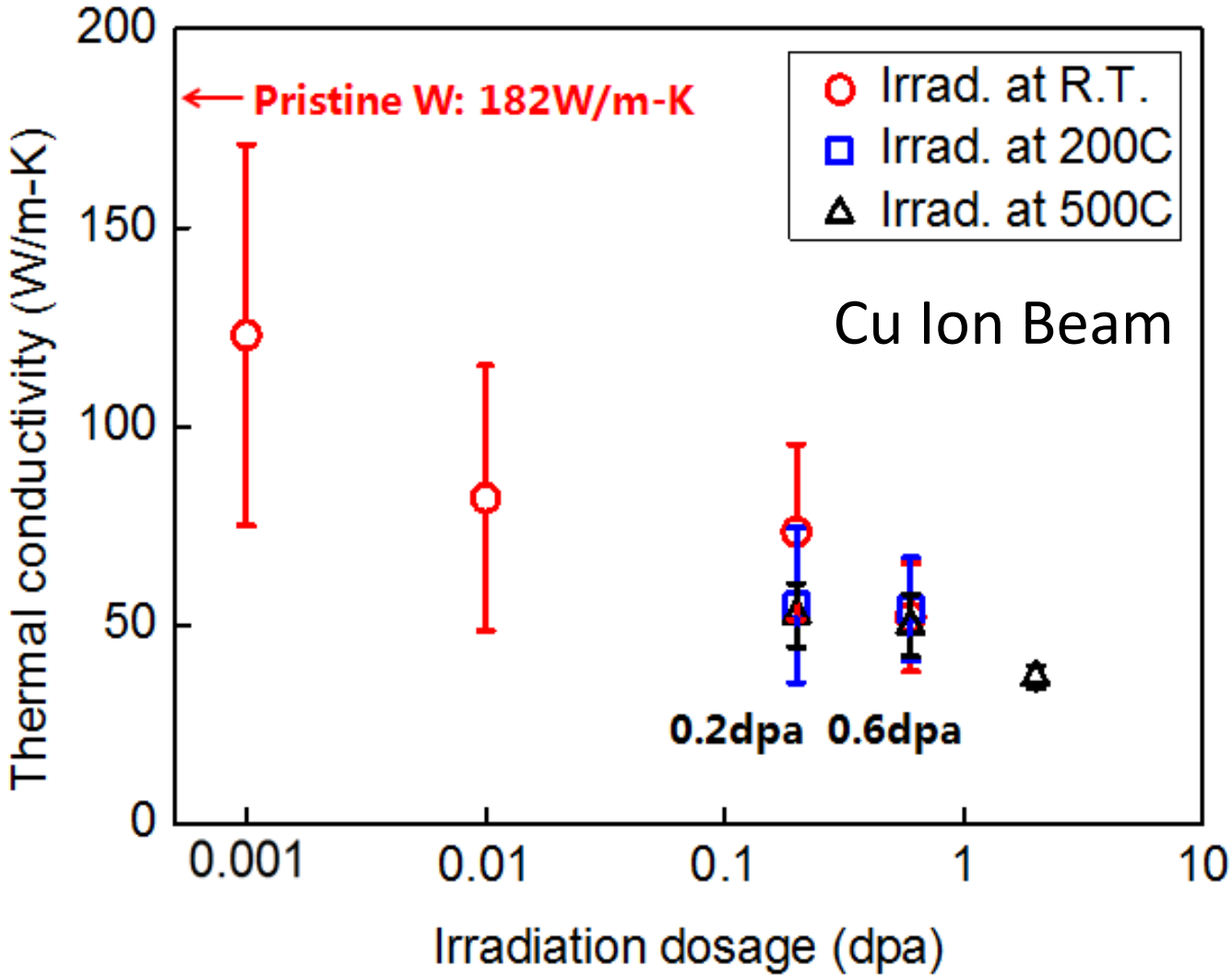
κ of the plasma-irradiated W is independent of the temperature for 300-500 K, indicating **defect-induced electron scattering dominates thermal conductivity**

Room-temperature displacement damage leads to ***significant reduction*** in thermal conductivity



S. Cui, R. Chen et al, in prep.

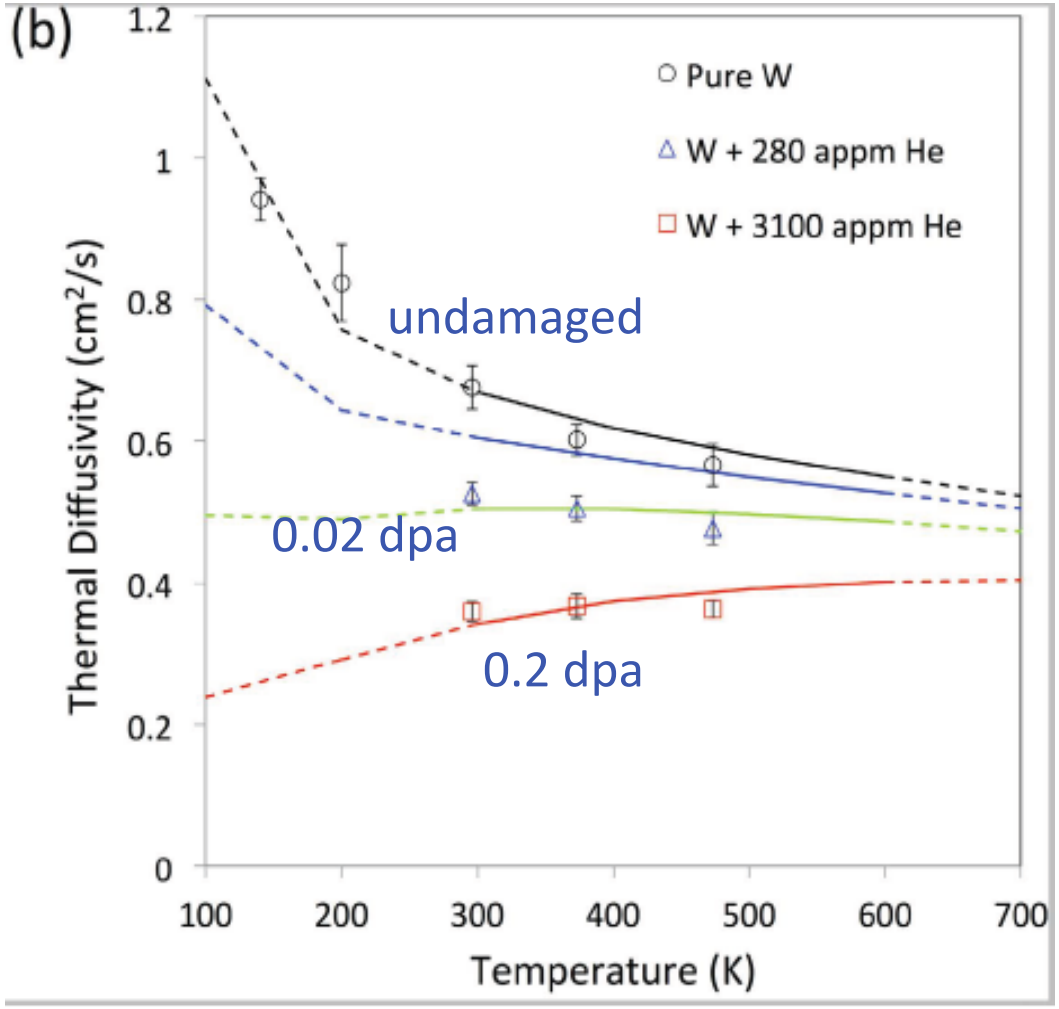
Reduced thermal conductivity also seen with high temperature displacement damage



S. Cui, R. Chen et al, in prep.

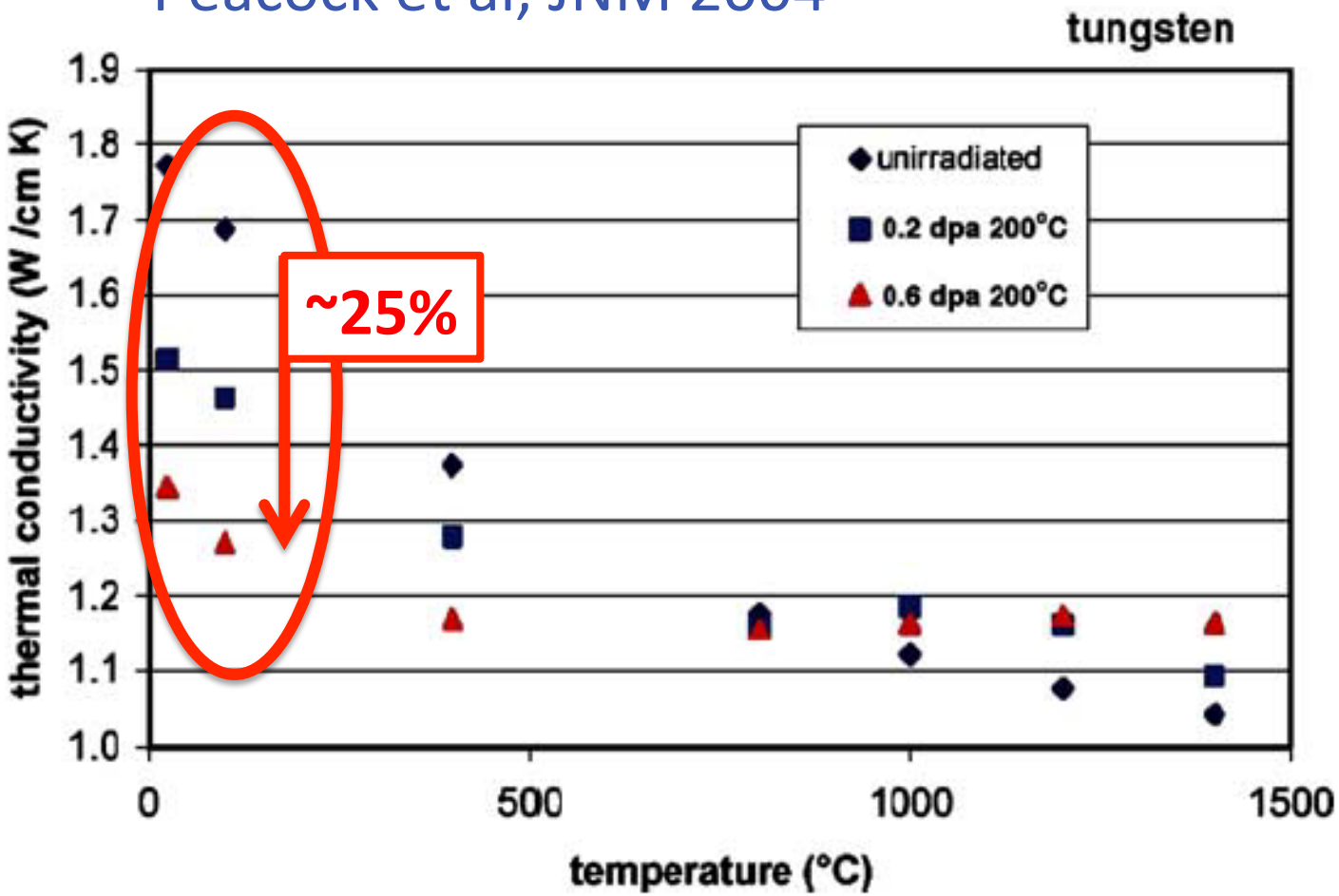
Comparable reduction w/ He ion beam damage

Hofmann, Nature-Sci Reports 2015

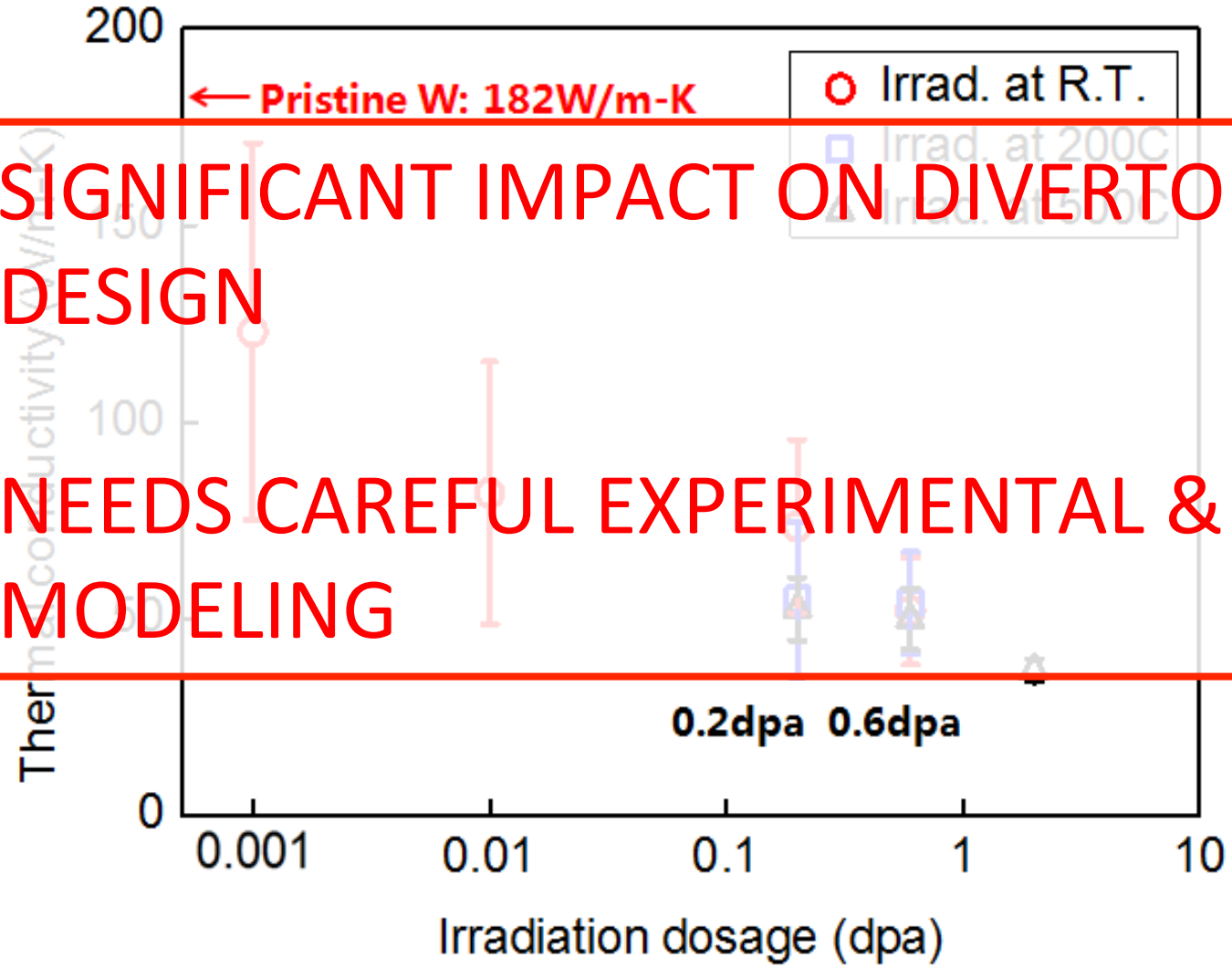


More modest reductions reported in fission-reactor irradiations

Peacock et al, JNM 2004



Reduced thermal conductivity also seen with high temperature damage



SIGNIFICANT IMPACT ON DIVERTOR DESIGN

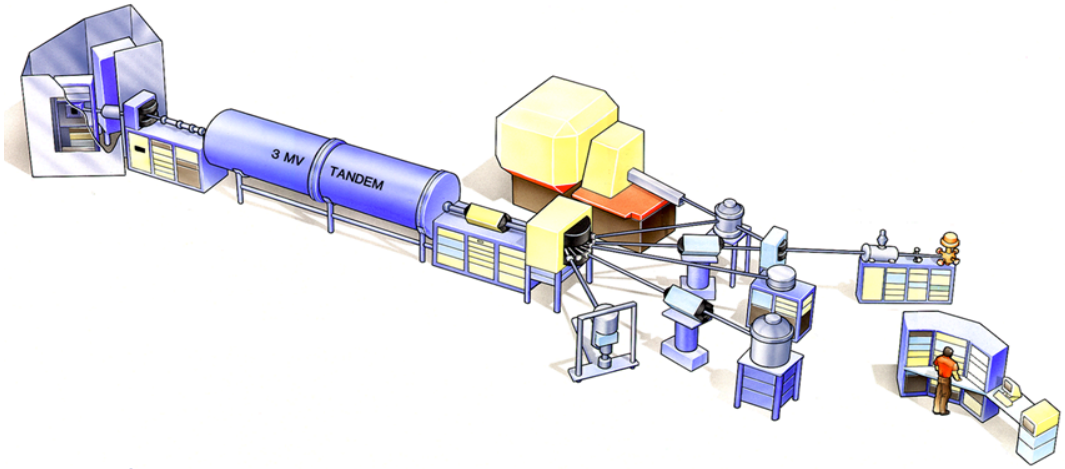
NEEDS CAREFUL EXPERIMENTAL & MODELING

S. Cui, R. Chen et al, in prep.

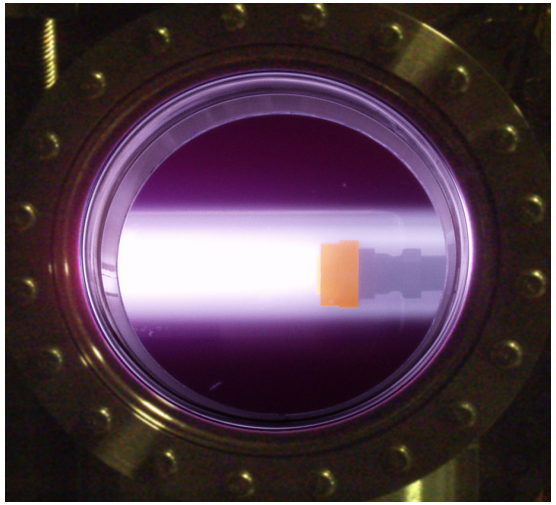
D retention in displacement-damaged W

PISCES

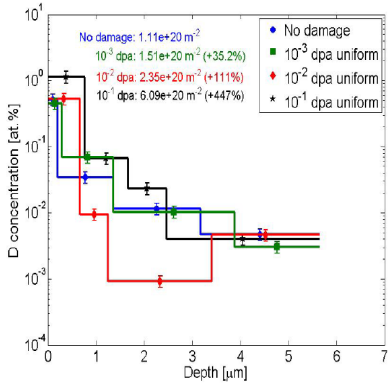
1) Induce Damage w/ Heavy Ion Beams

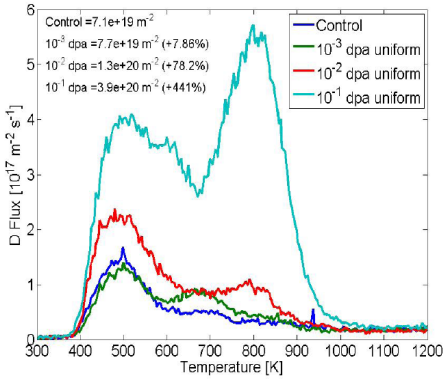


2) Implant D in Plasma Device

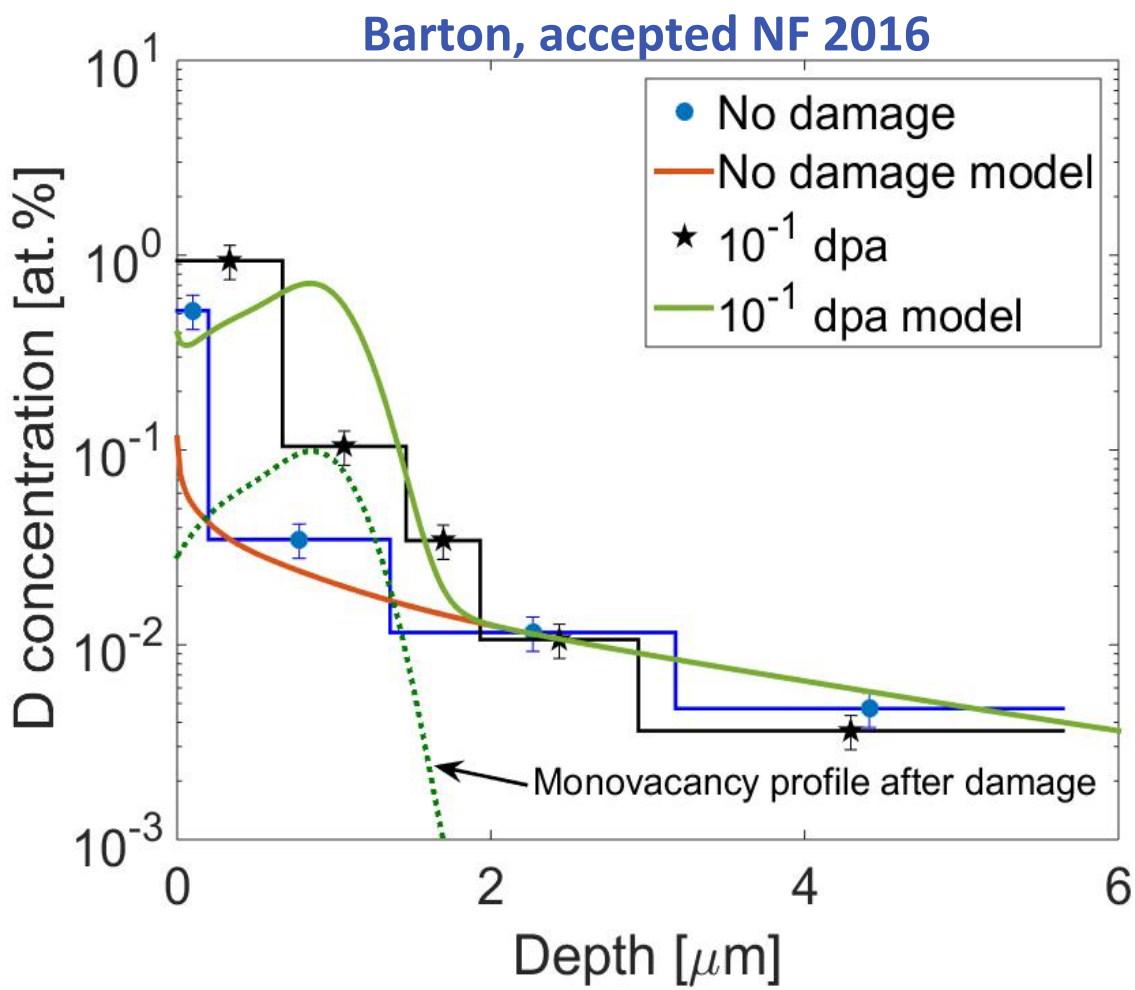


3) Measure D profile, content





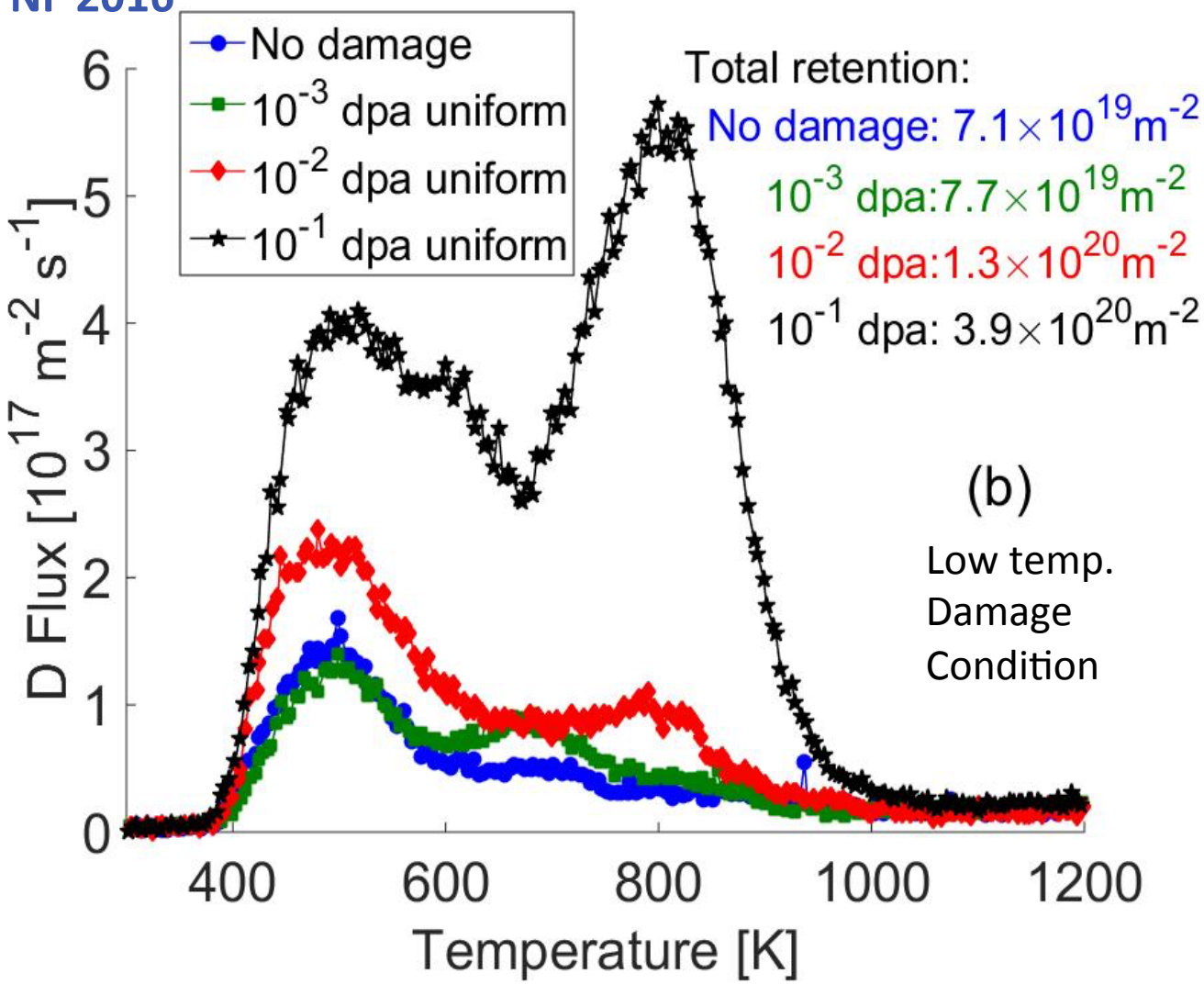
Experiment & modeling show increased retention & deeper diffusion in damaged W



See e.g. Arkhipov'07, Oliver&Causey'04, Fukumoto'09, Wampler&Doerner'09

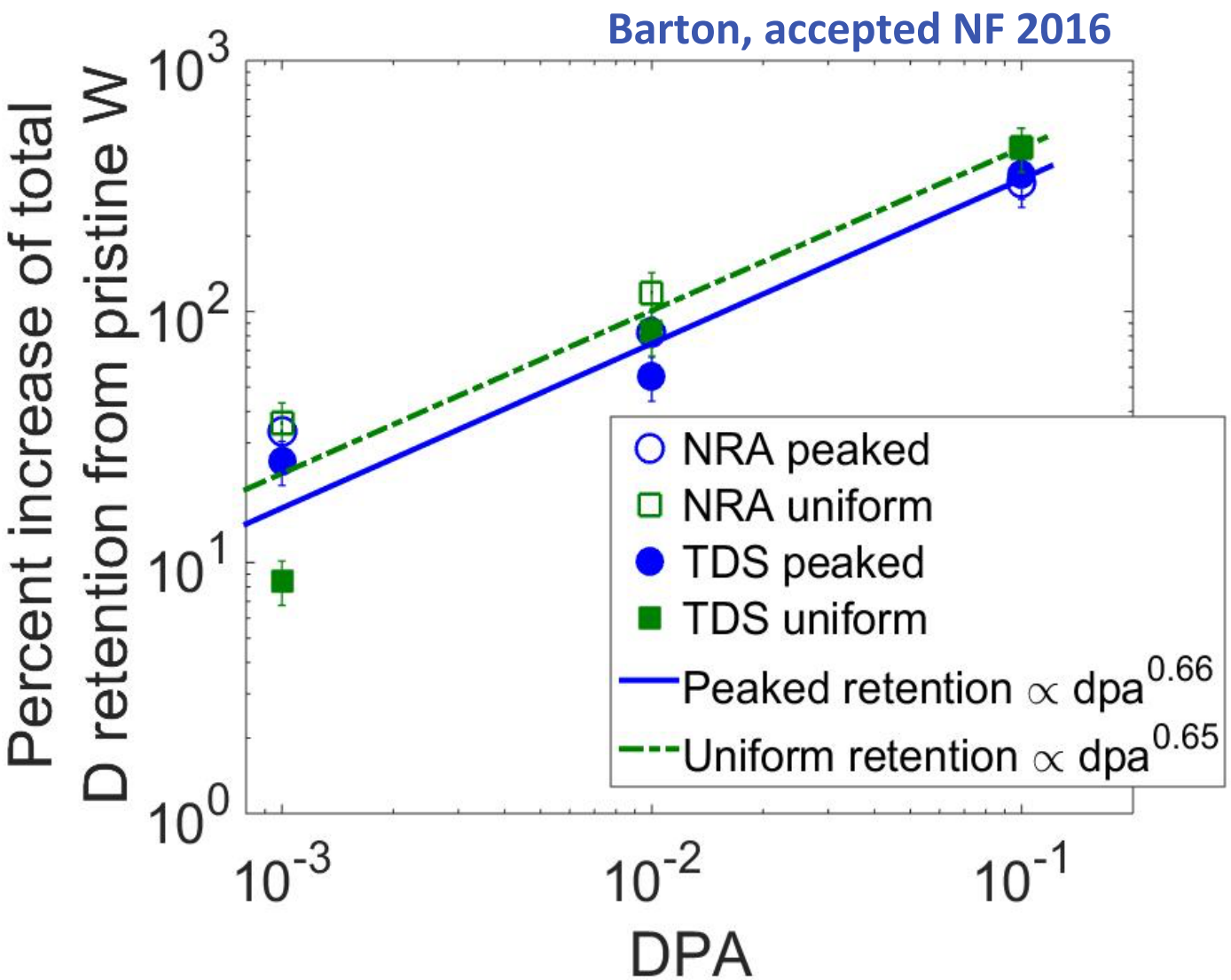
Increased retention occurs in deeper traps that release D at higher temperature

Barton, accepted NF 2016



See e.g. Arkhipov'07, Oliver&Causey'04, Fukumoto'09, Wampler&Doerner'09

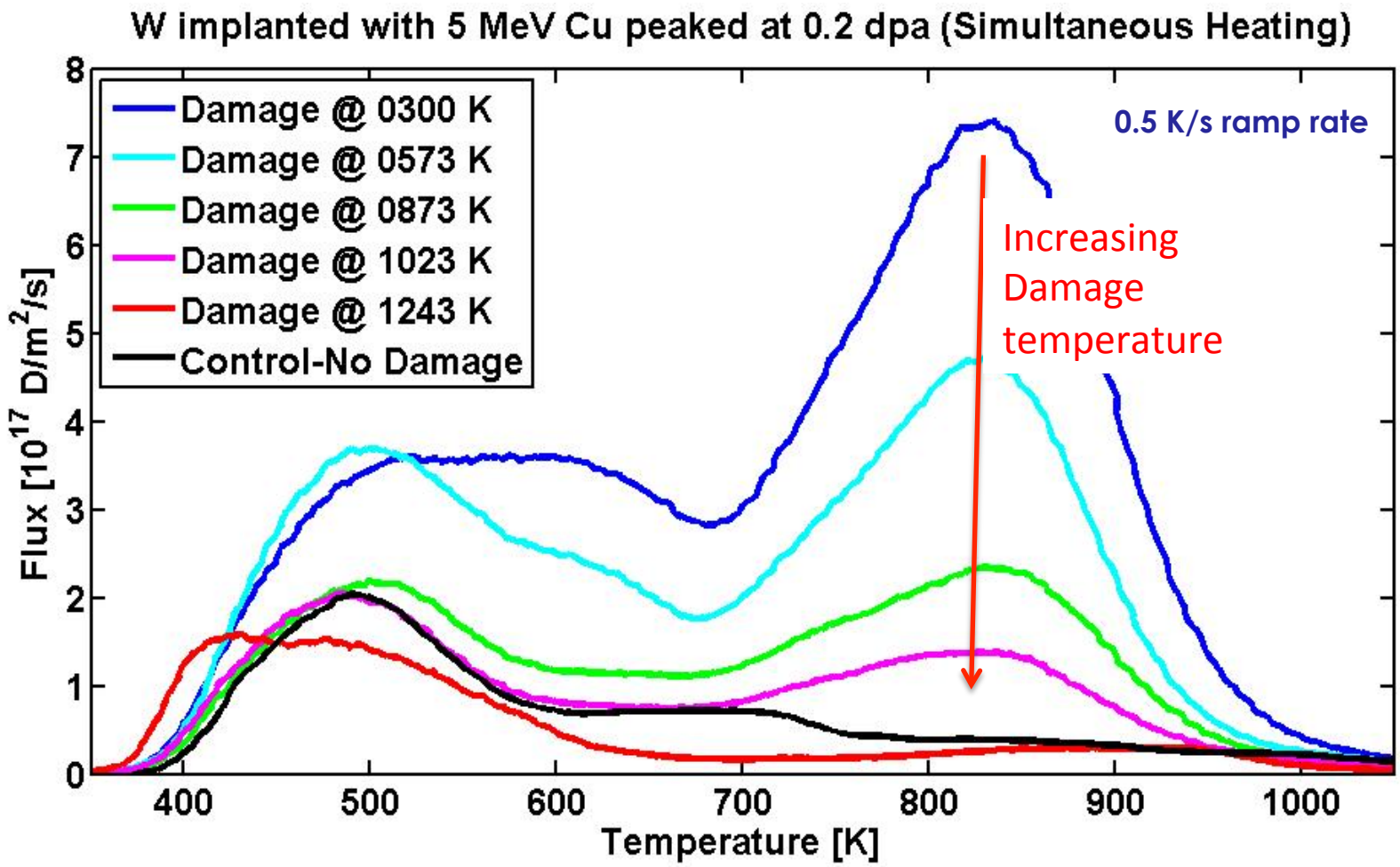
Retention increase proportional to dpa$^{0.65}$



See e.g. Tuburska'09, Wright'10, t'Hoen'13

Decreased retention at high damage temperature: Annealing effects?

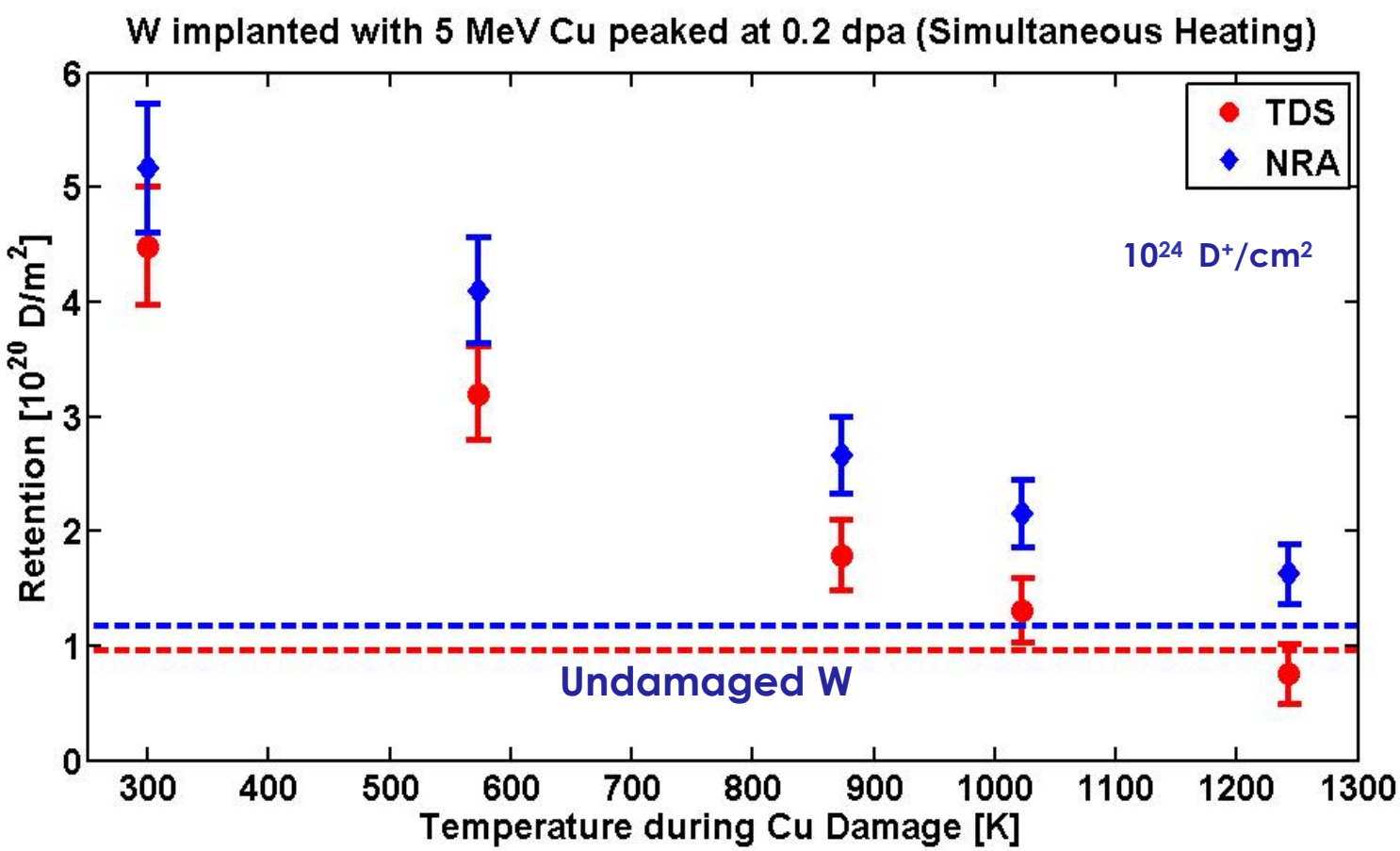
M. Simmonds, in prep. 2016



See e.g. Oliver&Causey'04, Wright'10, Ogorodnikova'14

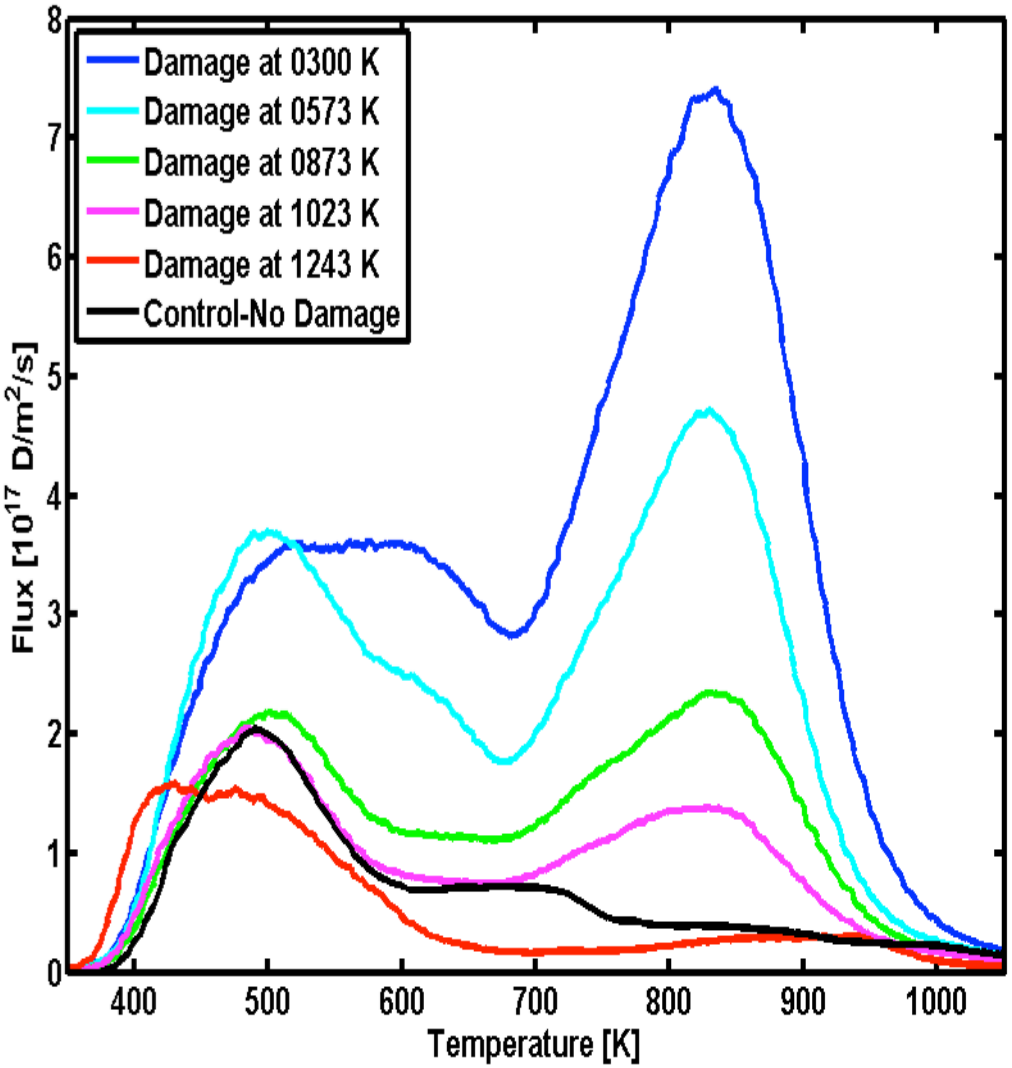
Undamaged retention recovered in high temperature damaged W

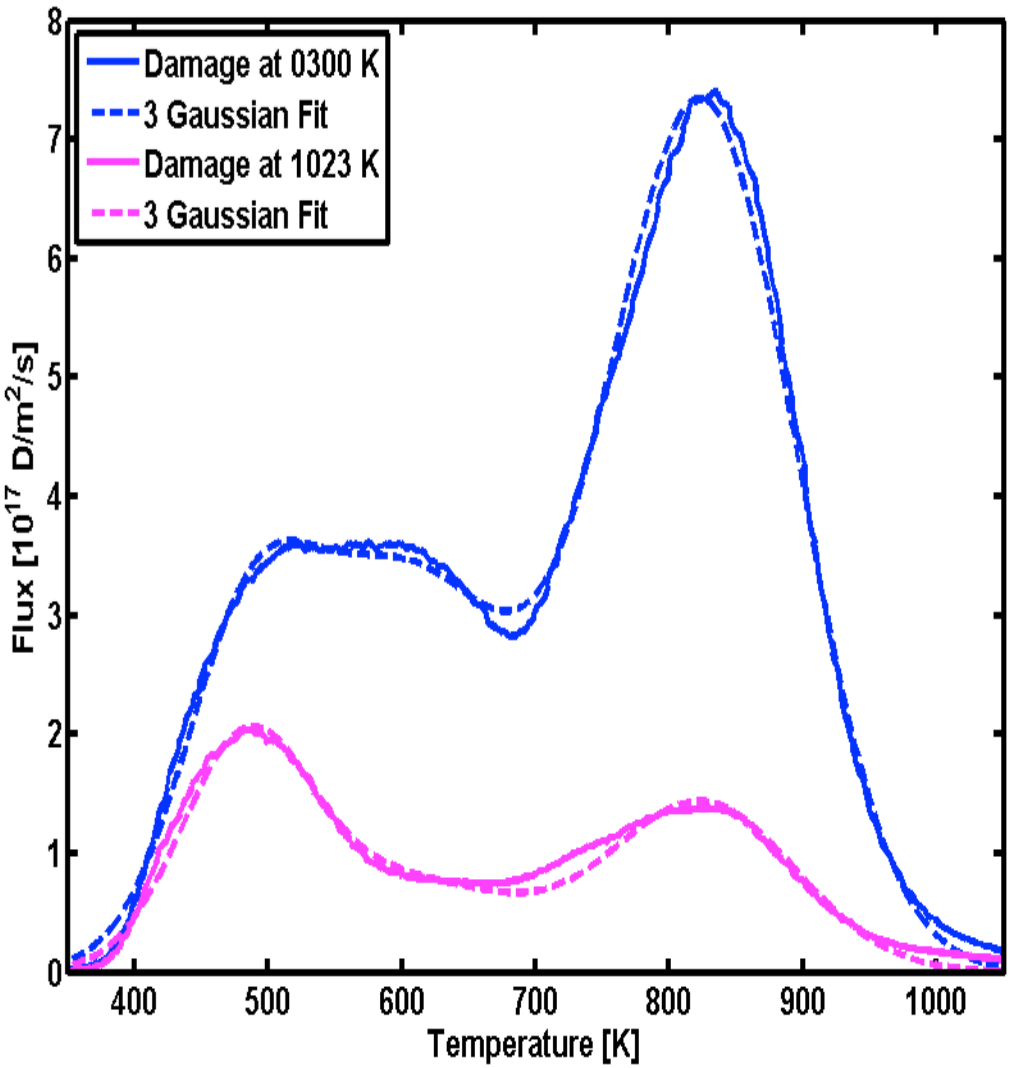
M. Simmonds, in prep. 2016



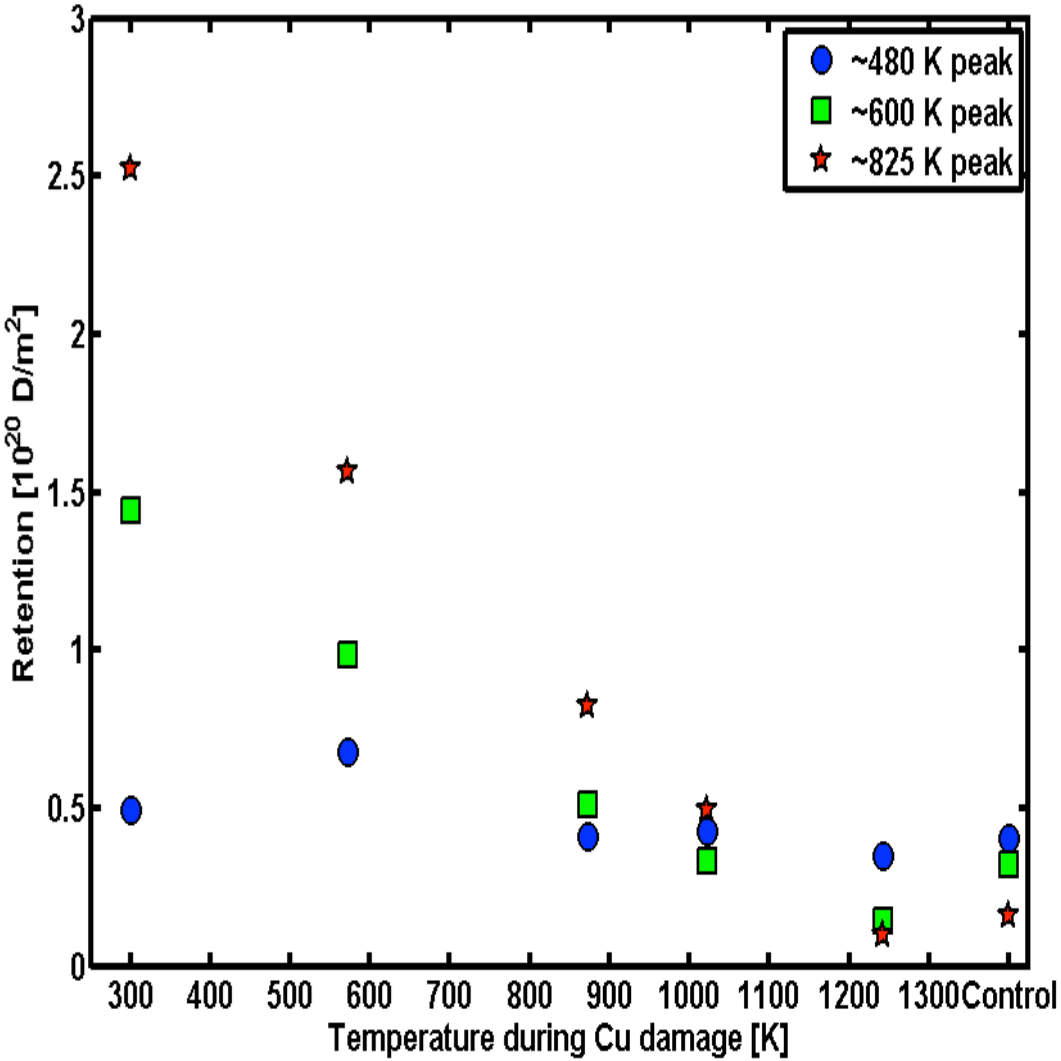
See e.g. Oliver&Causey'04, Wright'10, Ogorodnikova'14

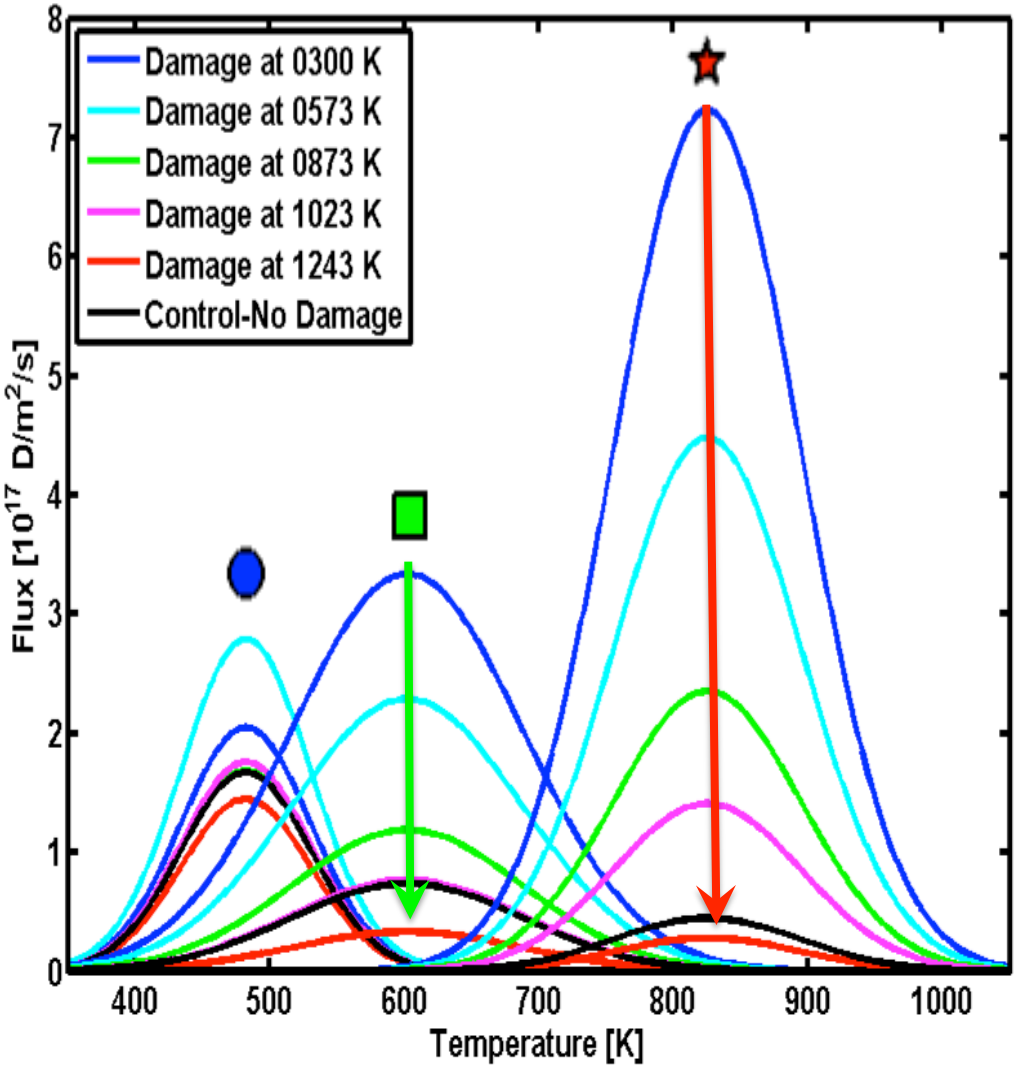
3 Gaussians were fit to each TDS profile



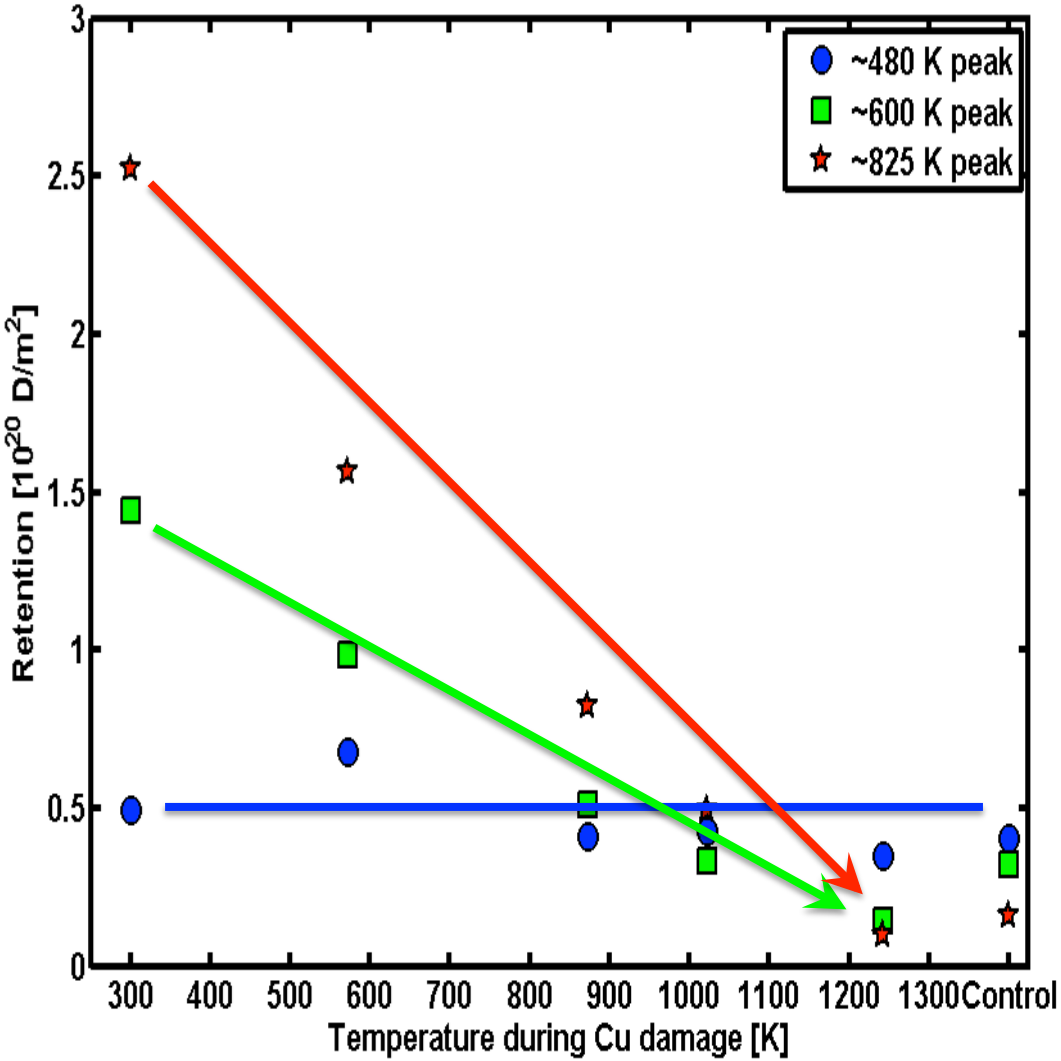


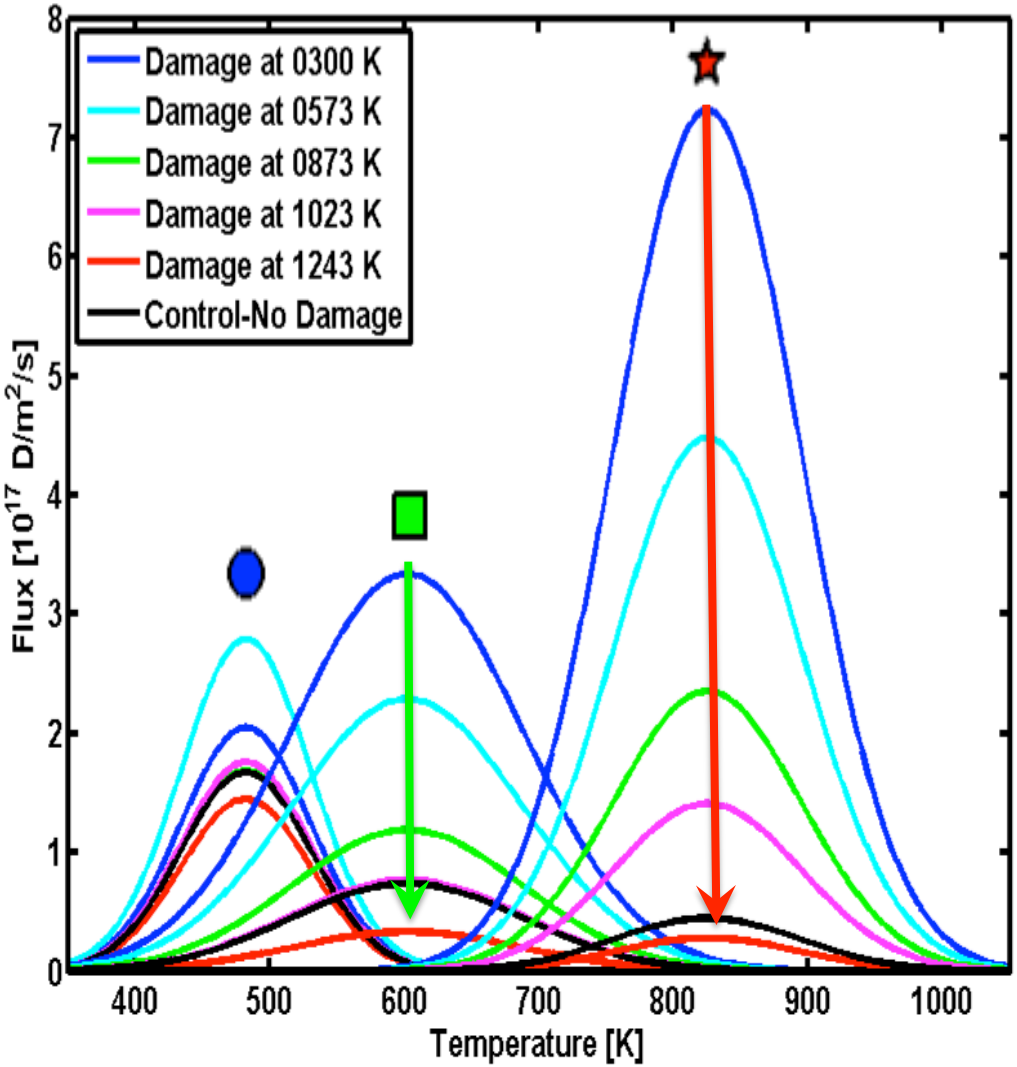
600 and 825 K Peaks Decrease with Damaging Temp



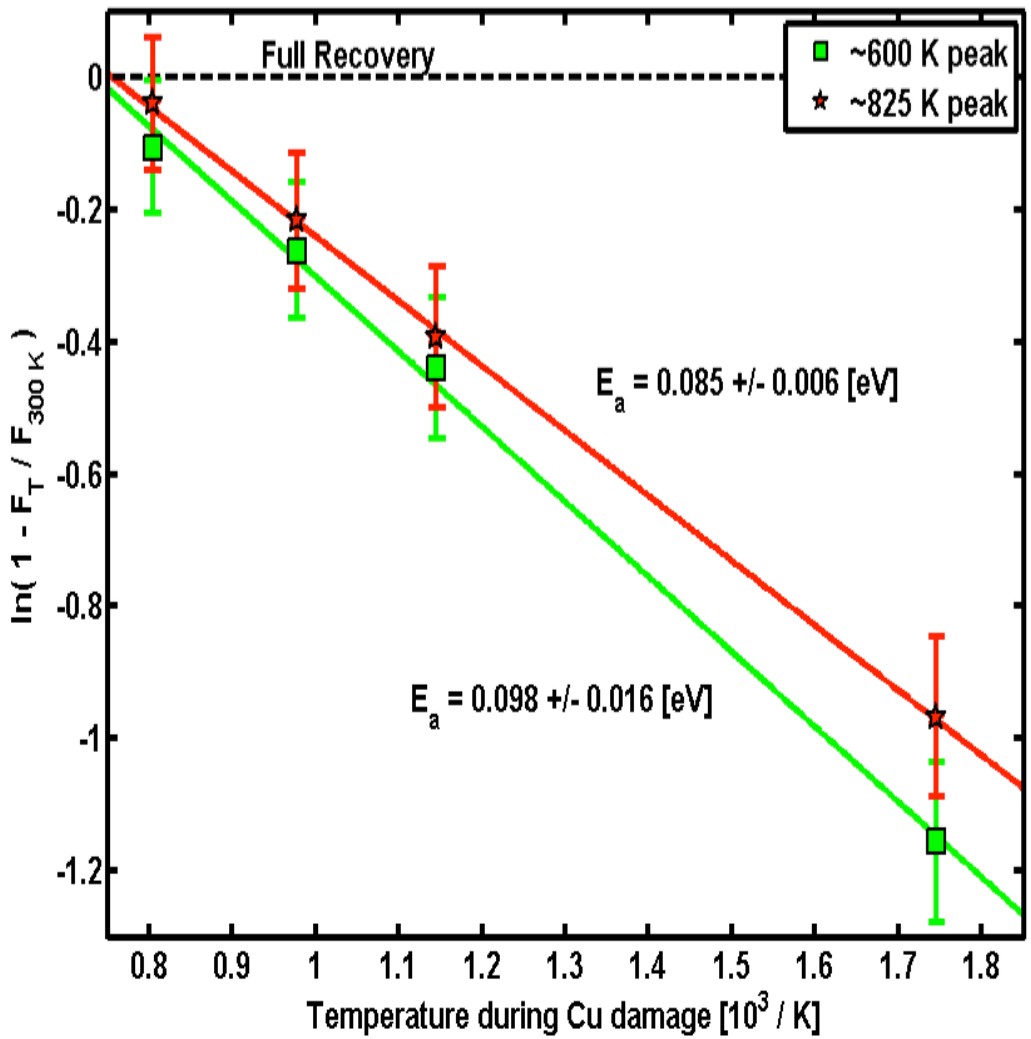


600 and 825 K Peaks Decrease with Damaging Temp



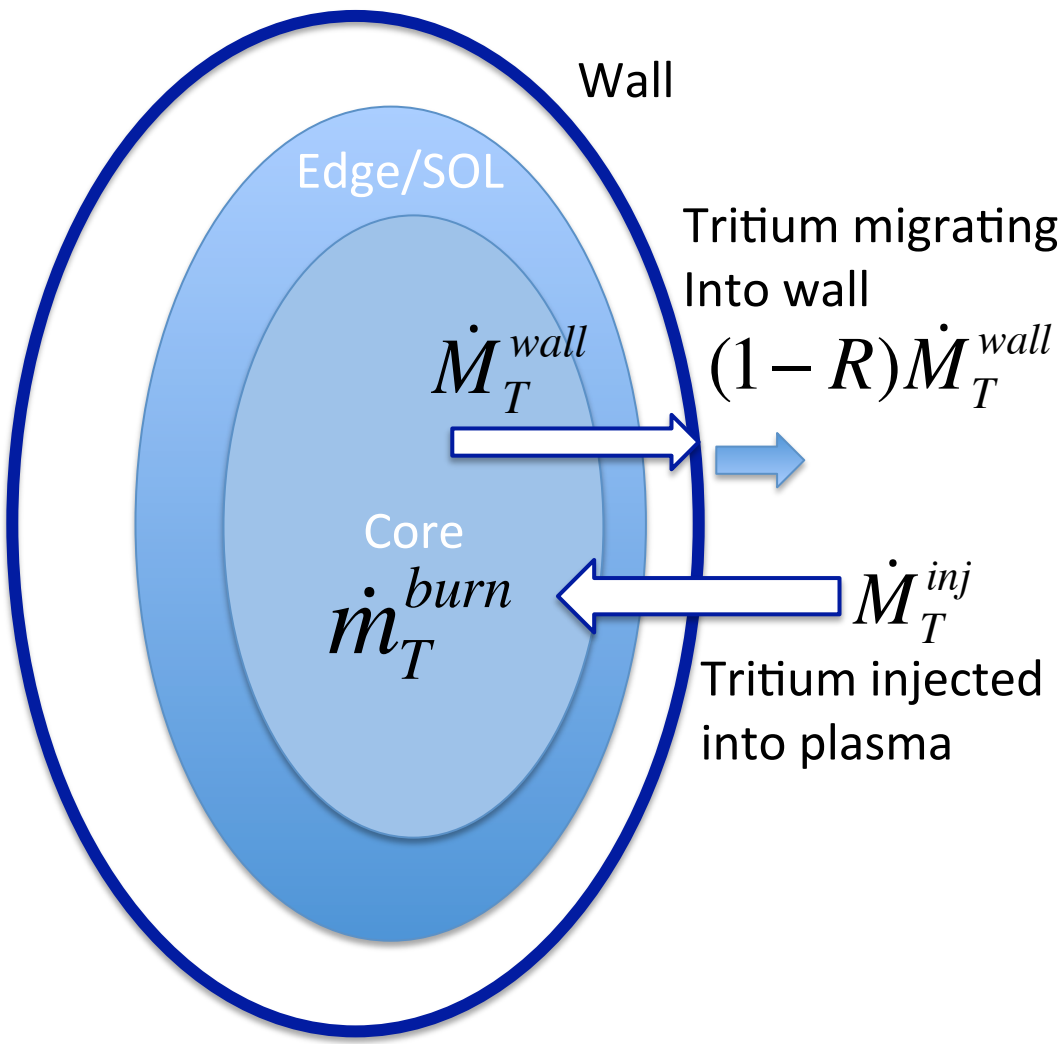


Experiments Give Activation Energy for Damage Recovery Mechanism



Implications for Tritium fuel cycle

Tritium Mass Balance



Define probability
of trapping T in wall, $p_{trap} = \dot{M}_T^{trap} / \dot{M}_T^{wall}$

$$p_{trap} << (TBR-1)(1-R)\frac{p_{burn}\eta_{fuel}}{1-p_{burn}\eta_{fuel}}$$

With typ. values

T burnup probability, p_{burn}~0.05

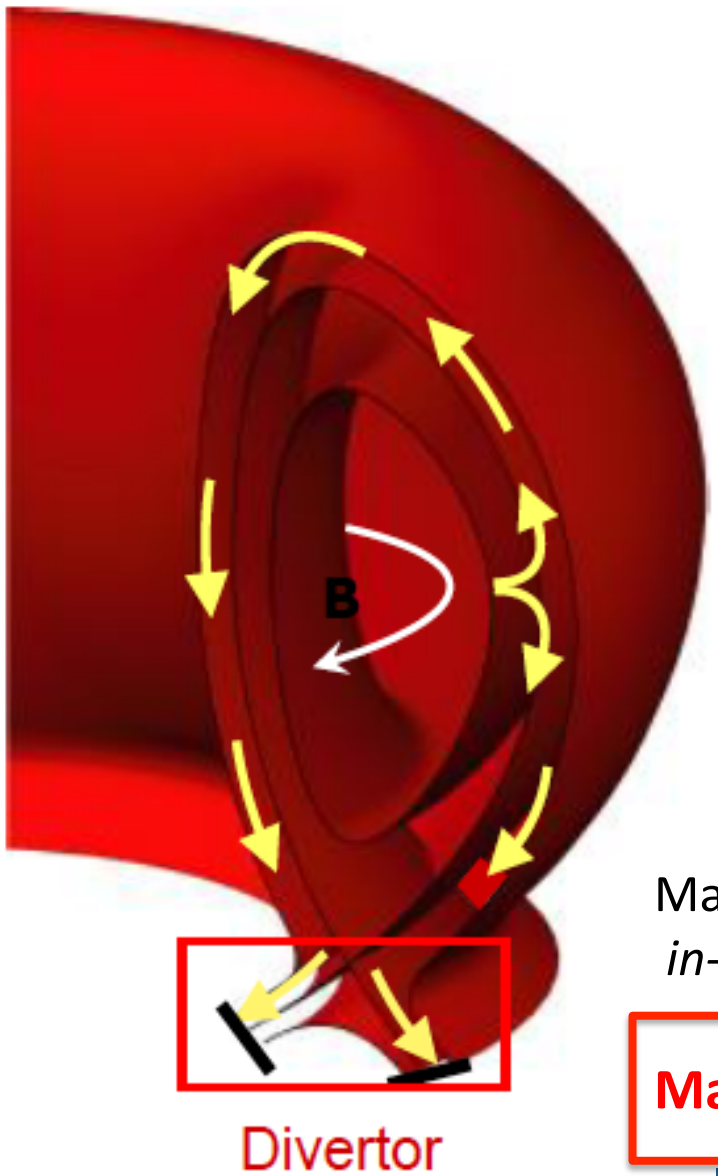
Fueling efficiency, η_{fuel}~20-30%

$$TBR \sim 1.05 \quad R \sim 0.99-0.999$$

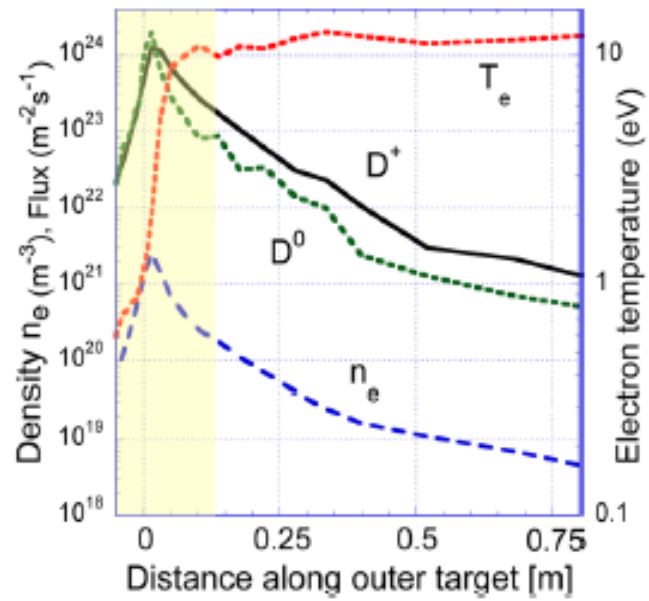
REQUIRES

$$p_{trap} << 10^{-6} - 10^{-7}$$

Implications for T inventory control



B2-Eirene Simulations, Kikushkin



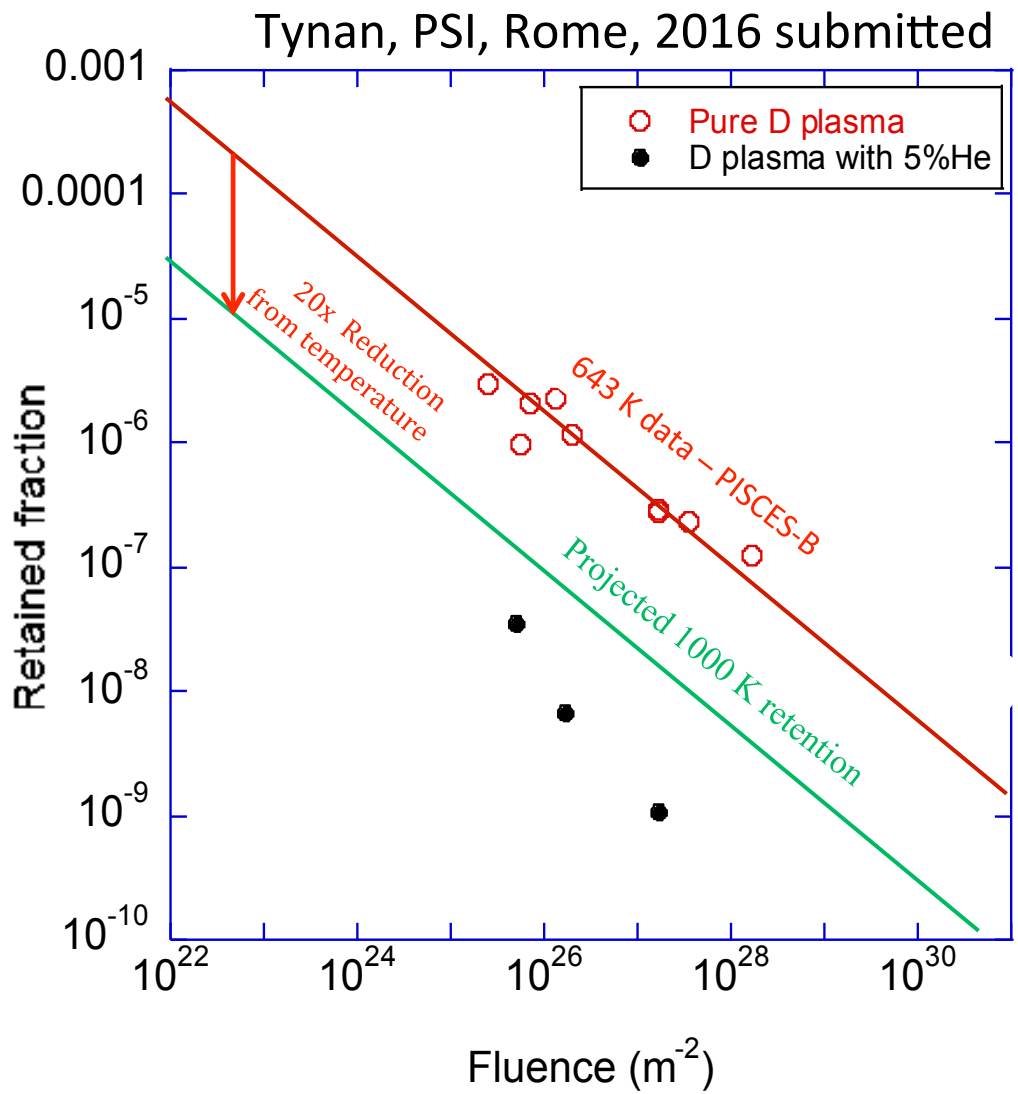
Particle Flux Into Divertor: ~10^{24}/m^2-sec ➔

Annual T fluence into divertor: 300 Tonnes-T/year

Maximum allowable mobilizable *in-vessel* T inventory: O(1kG)

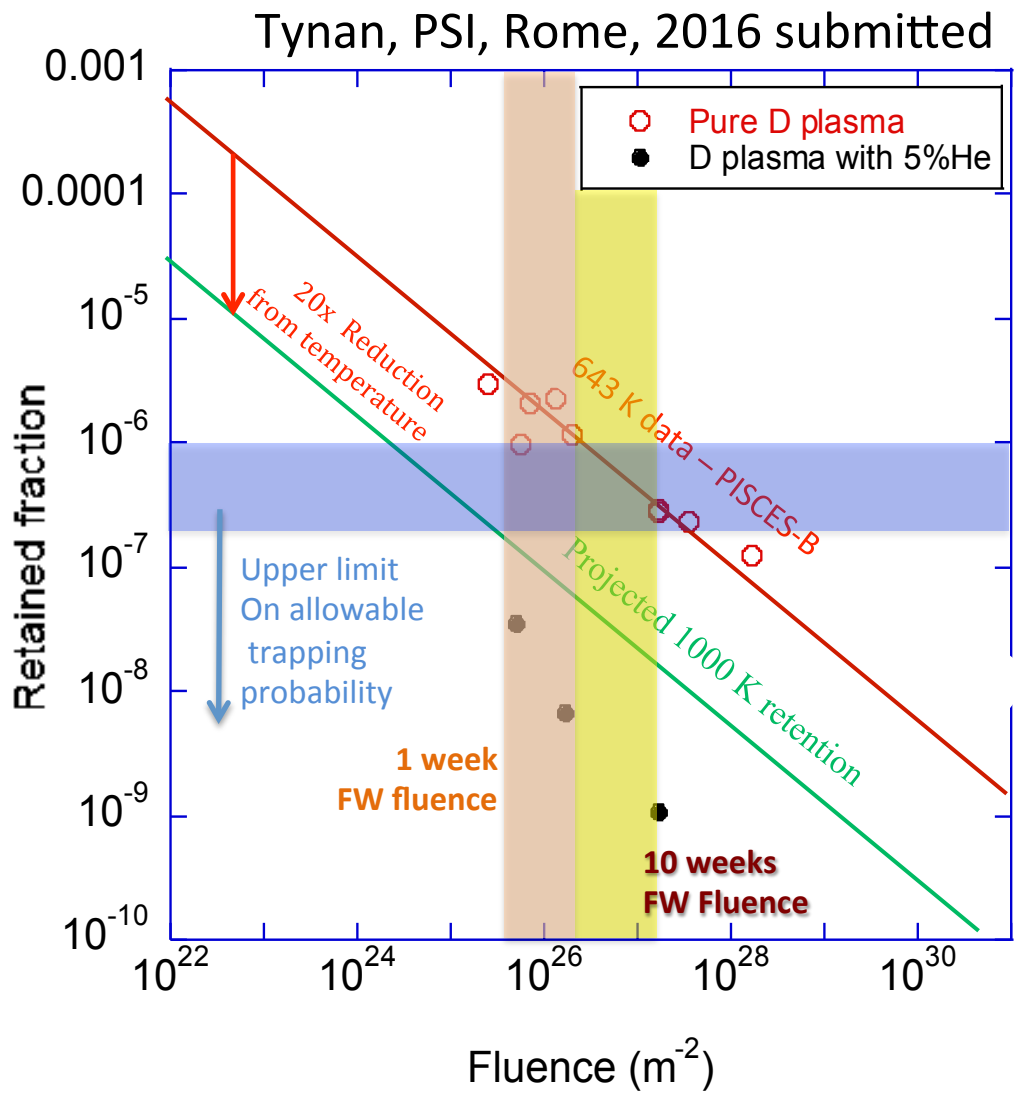
Maximum allowable T retention probability: 3×10^{-6}

Experiments in undamaged W show retention probability drops with fluence

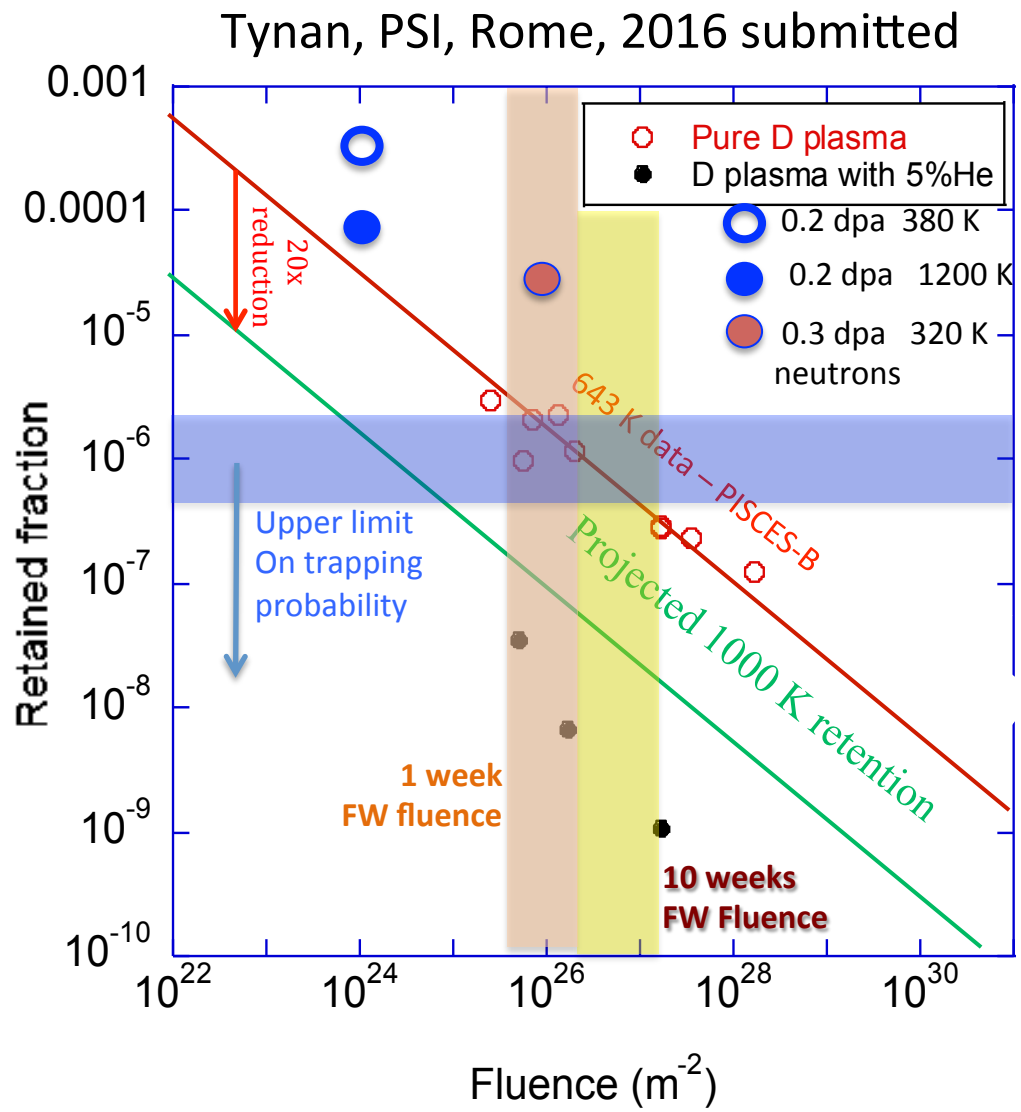


Based on data from
Doerner, in press, '16 & Baldwin, NF 2011

Observed Retention within limits in undamaged W

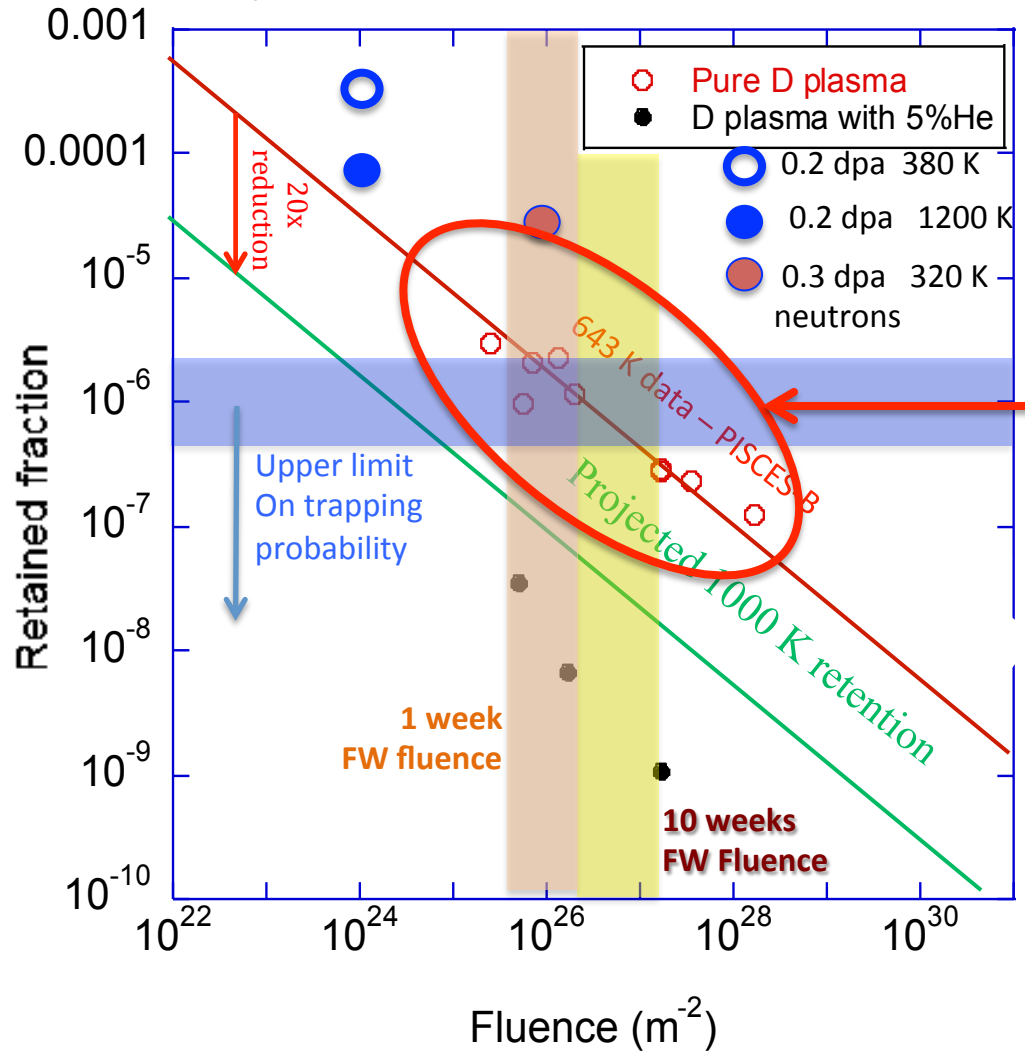


EXCESSIVE RETENTION in low-fluence damaged samples



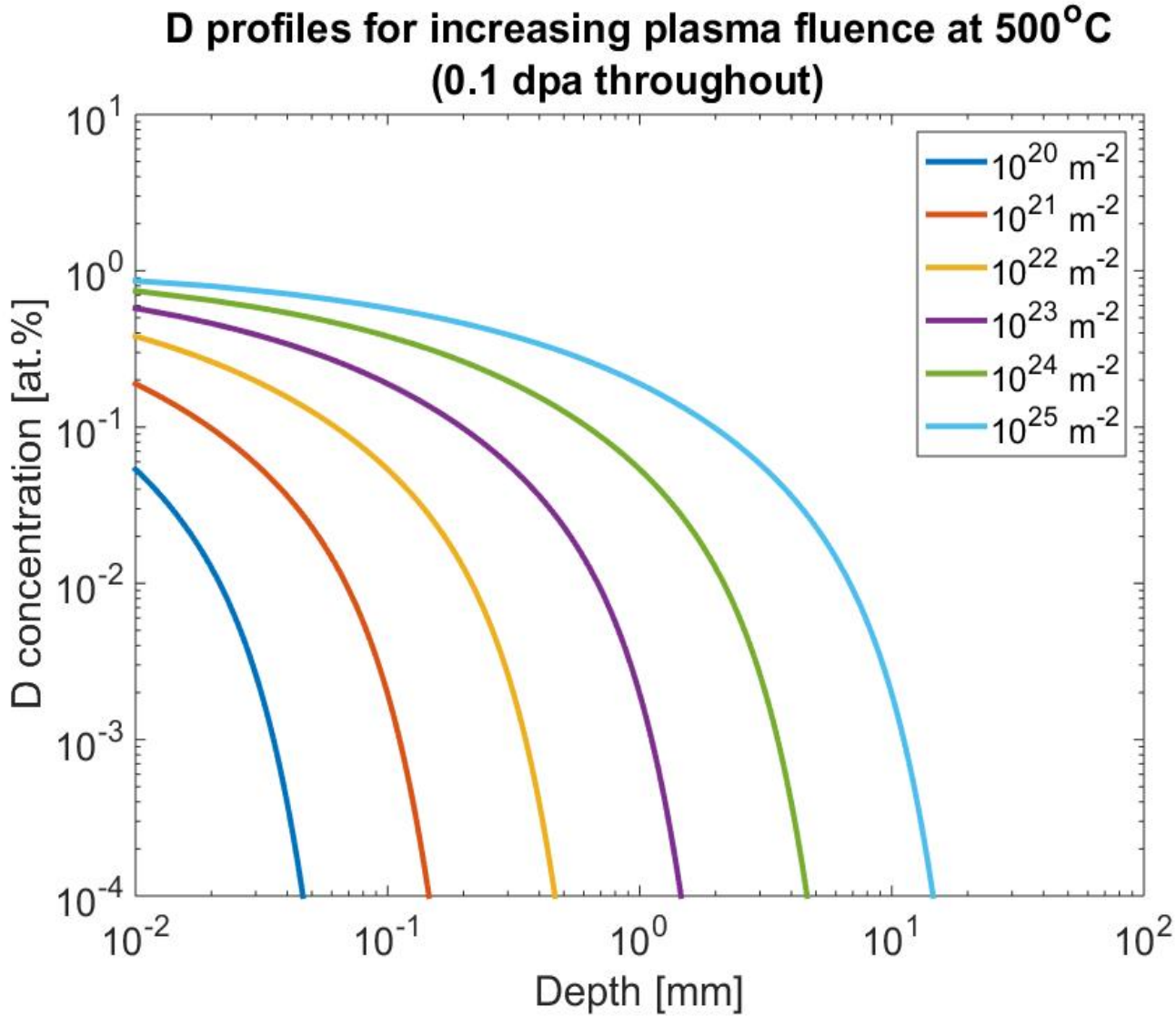
EXCESSIVE RETENTION in low-fluence damaged samples

Tynan, PSI, Rome, 2016 submitted



Need data
In damaged samples
With higher plasma
Fluence….

Modeling suggests deep penetration w/ significant retained inventory at low dpa



EXCESSIVE RETENTION in low-fluence damaged samples

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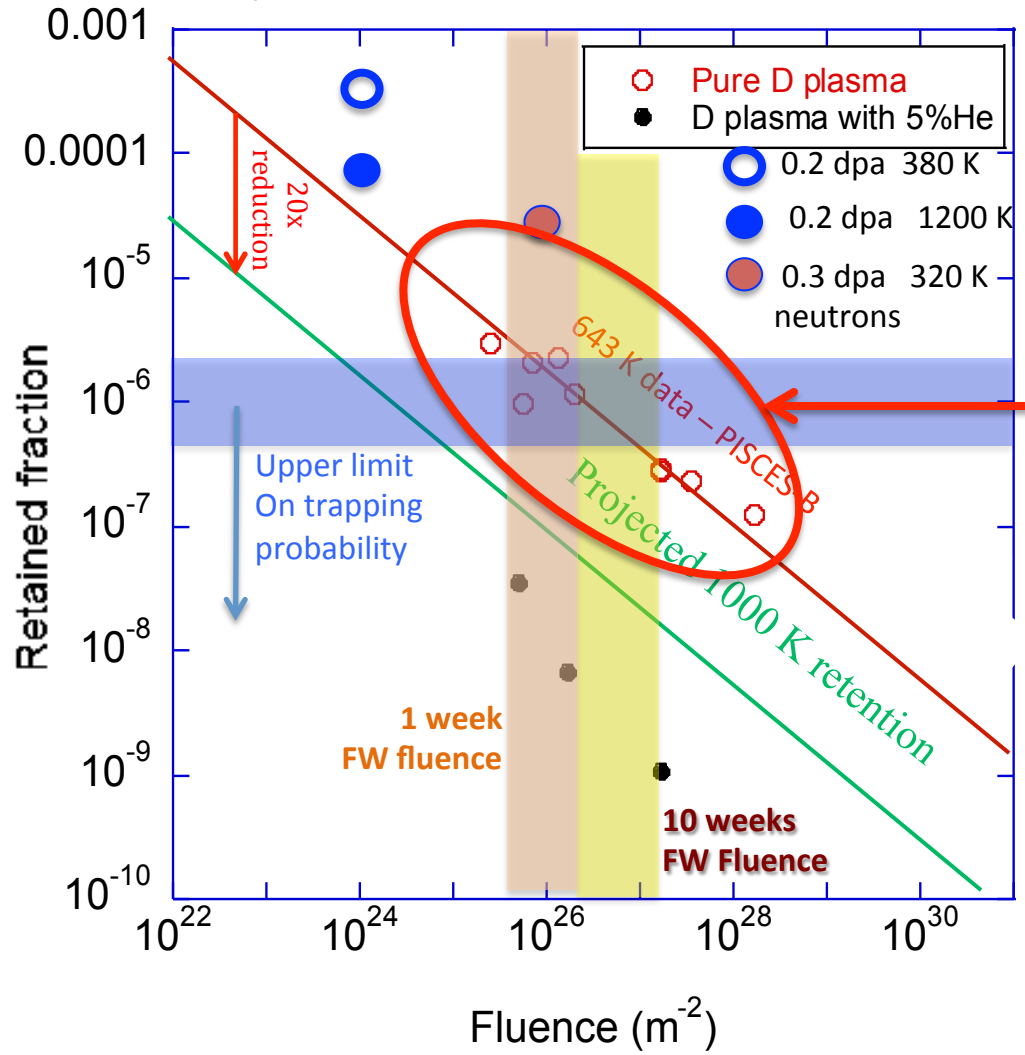
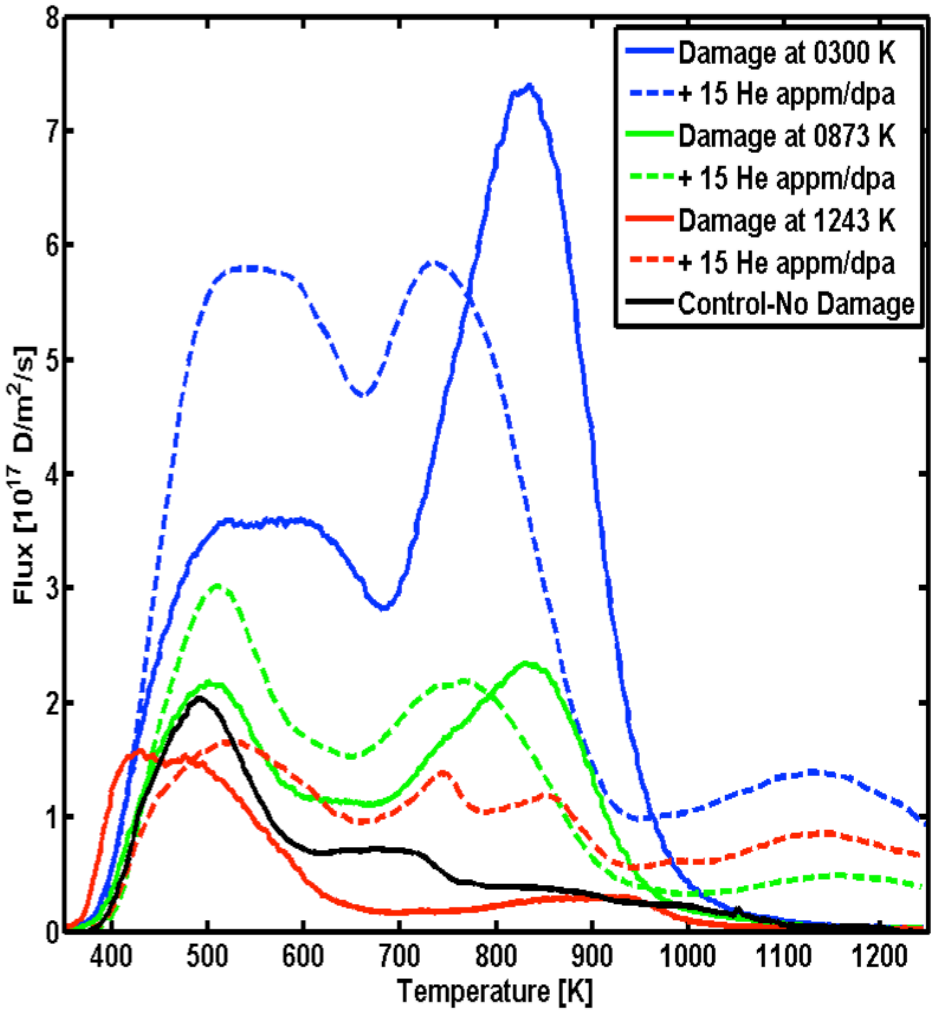


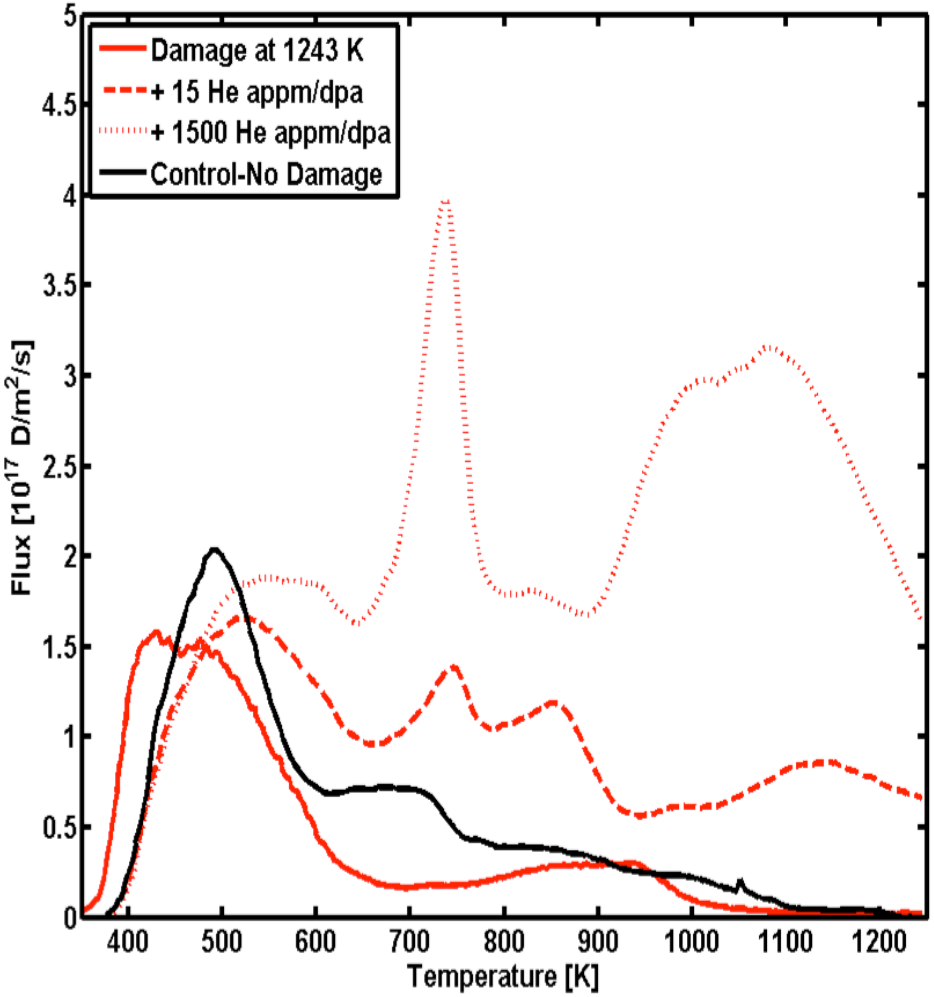
Motivates
Higher Plasma Fluence
Ion Beam Expts
AND
Neutron Irradiated
Samples

Preliminary: Dual Beam (He+Cu) **Experiments Suggest Annealing Effects Will Survive** (n,α) in PFCs



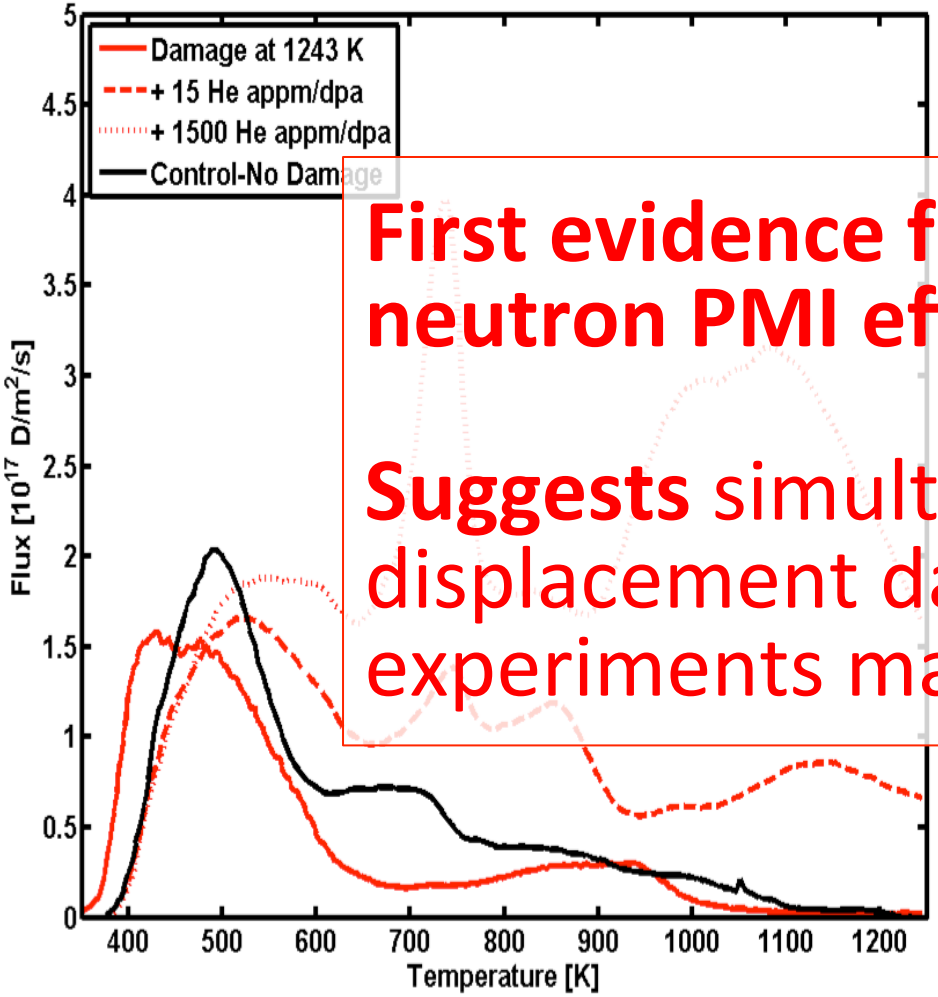
- Solid Lines - 5 MeV Cu up to 0.2 dpa (~0.9 um)
- Dashed Lines - 1.5 MeV Cu up to 0.35 dpa (~0.15 um) with 15 He appm/dpa (n-α)
- **TDS shows similar retention reduction (annealing)**

Preliminary: Dual Beam (He + Cu) Retention Suggests **Plasma-implanted He *Might* Influence Annealing** Effects



- 0 He appm/dpa (Cu damage only)
  - Retention approaches Control
- 15 He appm/dpa (n-α)
  - Does not approach intrinsic values
- 1500 He appm/dpa (plasma-implanted diffusion)
  - ~725 K & peaks above 1000 K grow
  - possibly due to He bubble formation
- Advanced TEM work by Dr. Parish underway

Preliminary: Dual Beam (He + Cu) Retention Suggests **Plasma-implanted He *Might* Influence Annealing** Effects



First evidence for synergistic plasma/ neutron PMI effects

Suggests simultaneous plasma/ displacement damage retention experiments may be important

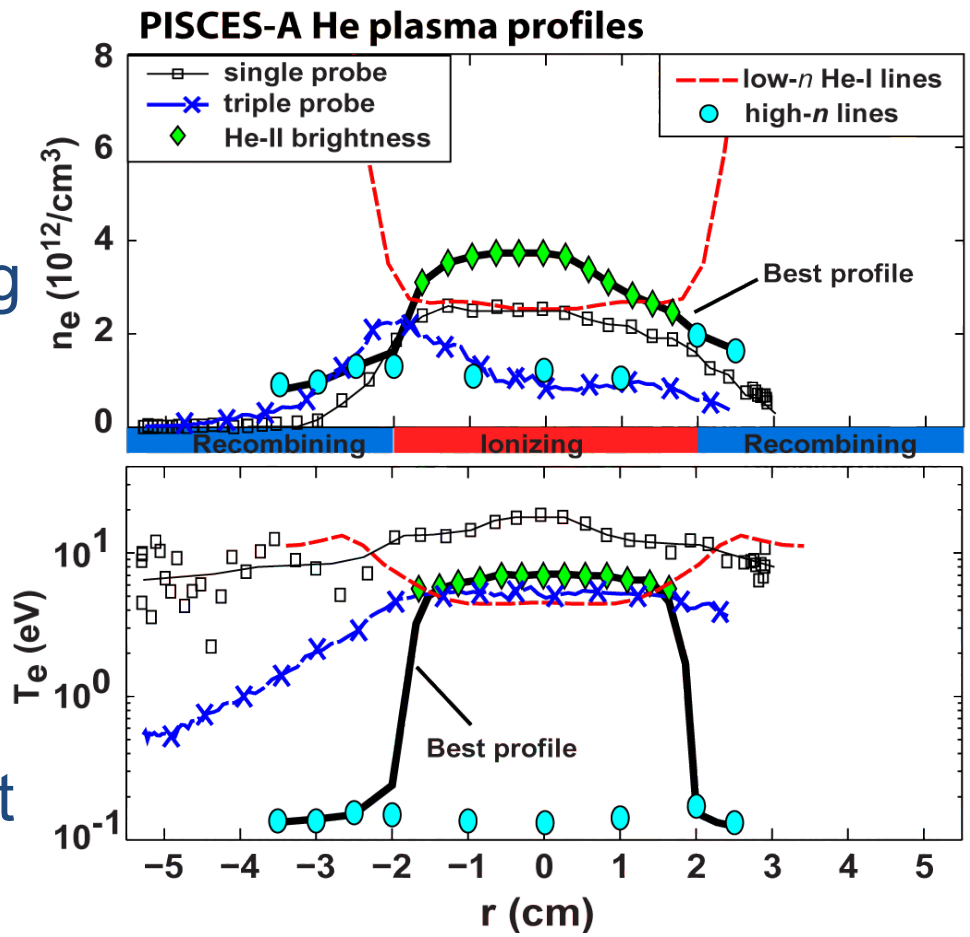
- 0 He appm/dpa (Cu damage only)
  - Retention approaches Control
- 15 He appm/dpa (n-α)
  - Does not approach intrinsic values
- 1500 He appm/dpa (plasma-implanted diffusion)
  - 723 K & peaks above 1000 K grow
  - possibly due to He bubble formation
- Advanced TEM work by Dr. Parish underway

PISCES Supporting Fusion Nuclear Science

- RAFM Steel Erosion Studies (w/ IPP-Garching)
- Plasma & displacement damage effects on PFC thermo-mechanical properties
- Displacement damage effects on D Retention & Removal (UC-funded collaboration w/ LANL)
- Simultaneous displacement damage/He production effects on D Retention
- **Divertor Physics, In-situ PMI Diagnostic Development**
- Material Migration Studies

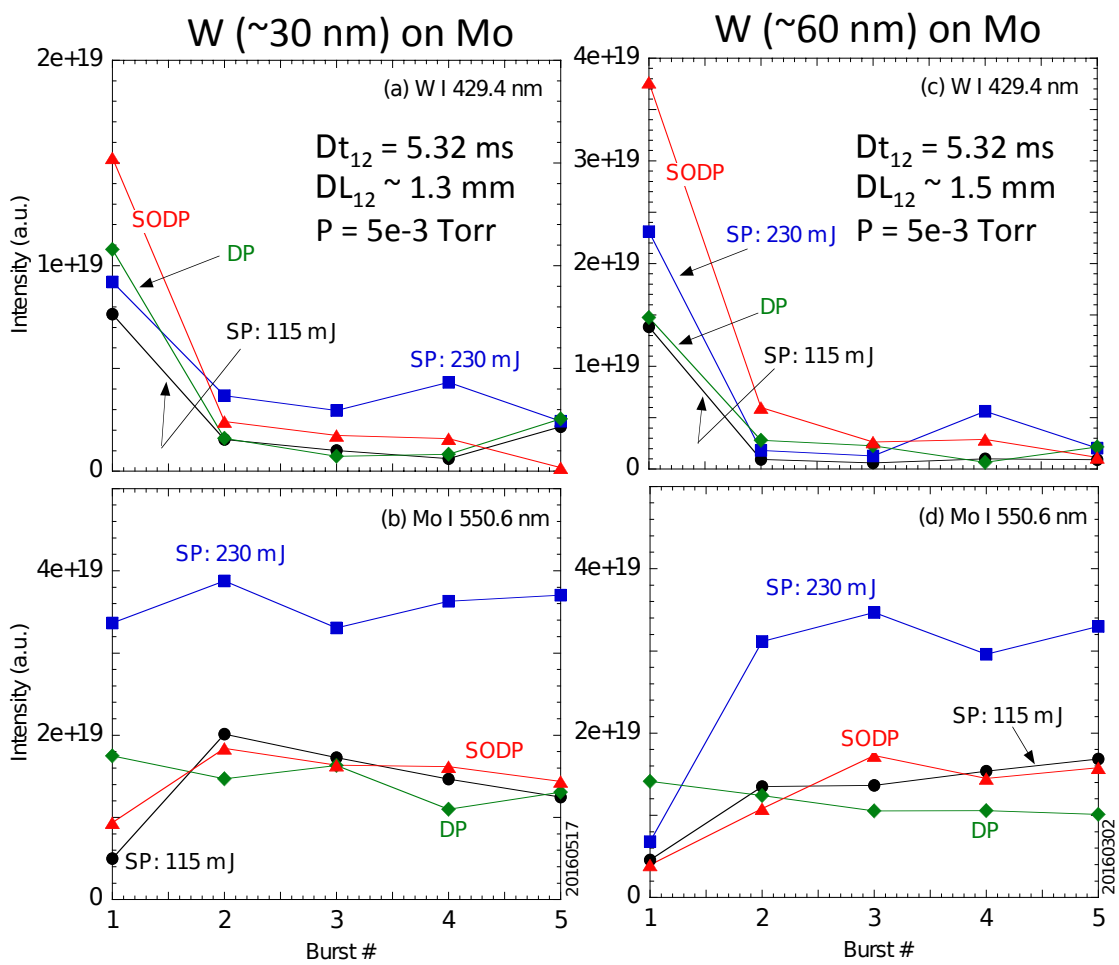
Pisces-A studies of spectroscopic diagnosis of ionizing + recombining divertor-like plasmas

- Ionizing plasma at r=0; recombining at r=a.
- Best results use high-*n* line He-I Boltzmann analysis in recombining region and He-II absolute brightness in ionizing region.
- Well-used He-I low-*n* line ratios method [Schweer 1992] gives extremely poor results in recombining region and somewhat better results in ionizing region (after including opacity correction [Nishijima 2007]).



A novel technique, spatially-offset double-pulse LIBS, has been invented for analysis of thin layers.

- **In SODP-LIBS, two laser spots are spatially offset by a few mm**, while there is no spatial gap for the standard collinear DP-LIBS.
- Compared to SP-LIBS and the standard collinear DP-LIBS,
  - **W I signal intensity is enhanced** with SODP-LIBS.
  - **A clearer transition between W and Mo** is obtained with SODP-LIBS.



PISCES Supporting Fusion Nuclear Science

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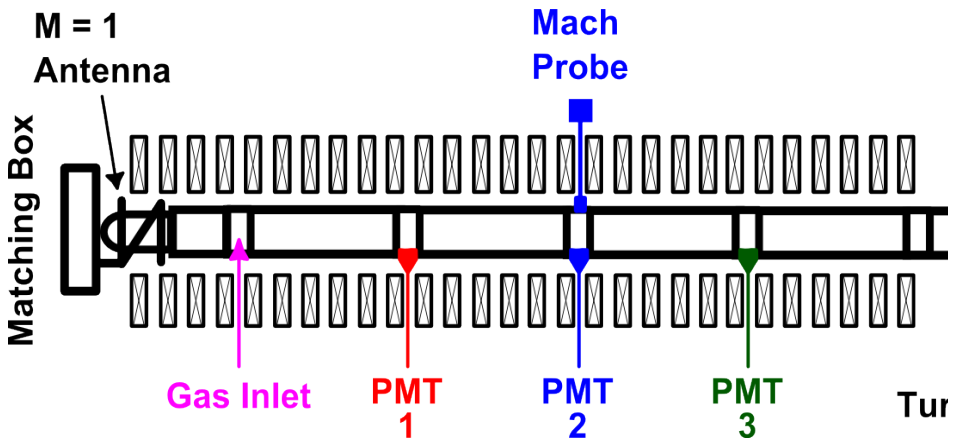
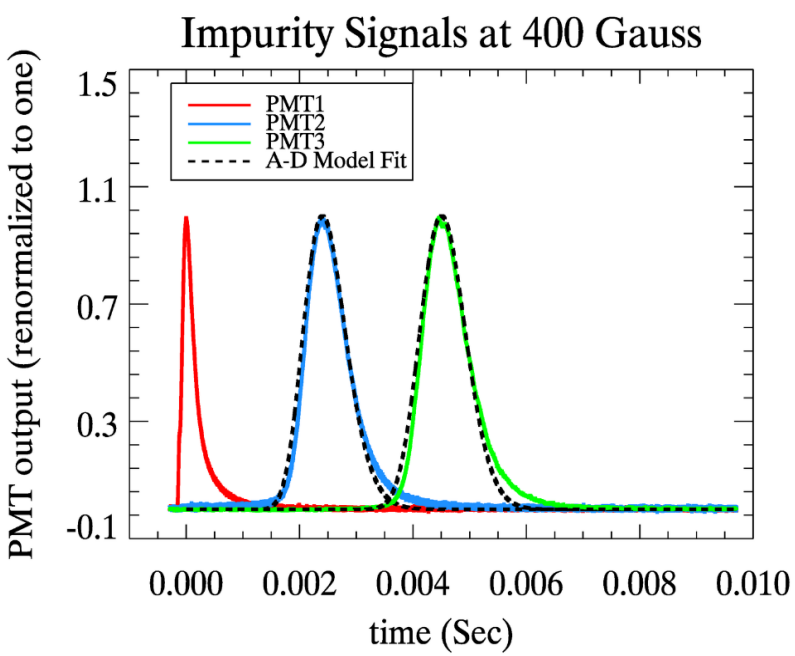
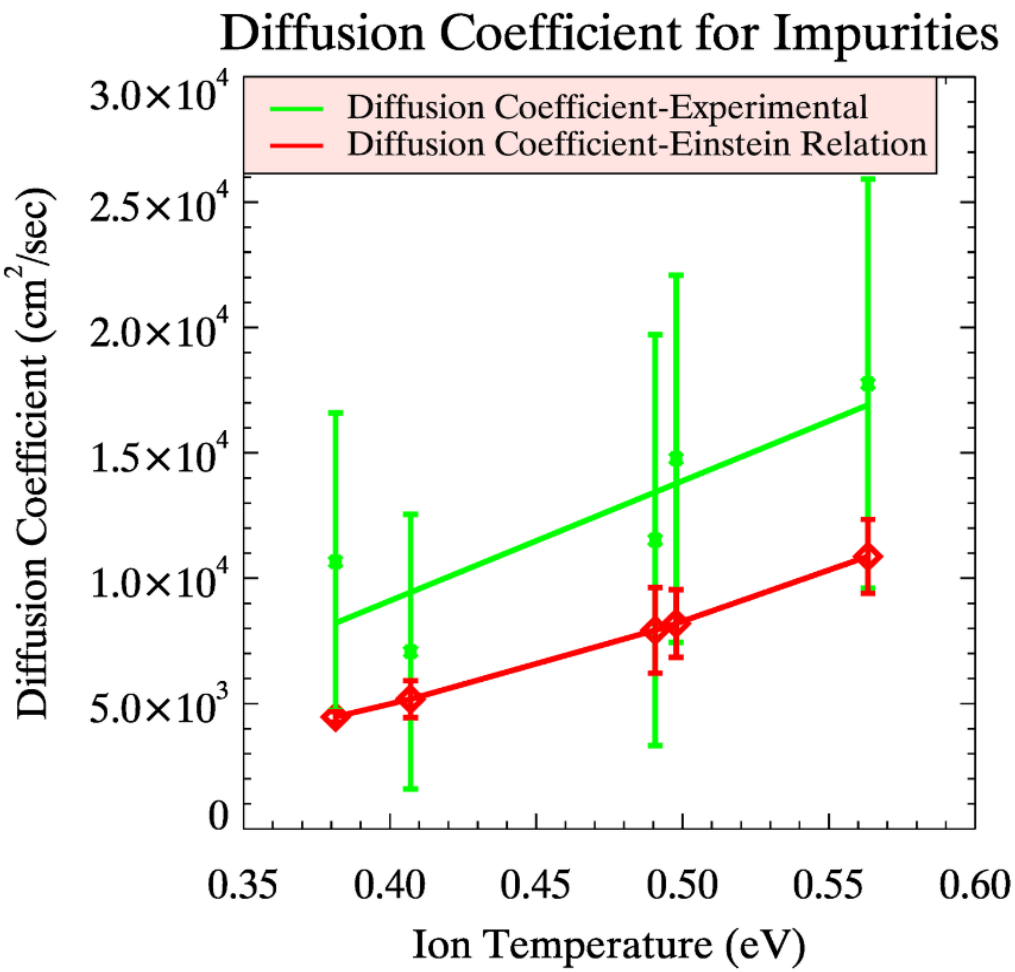
- **Material Migration Studies**

Parallel impurity diffusion is classical





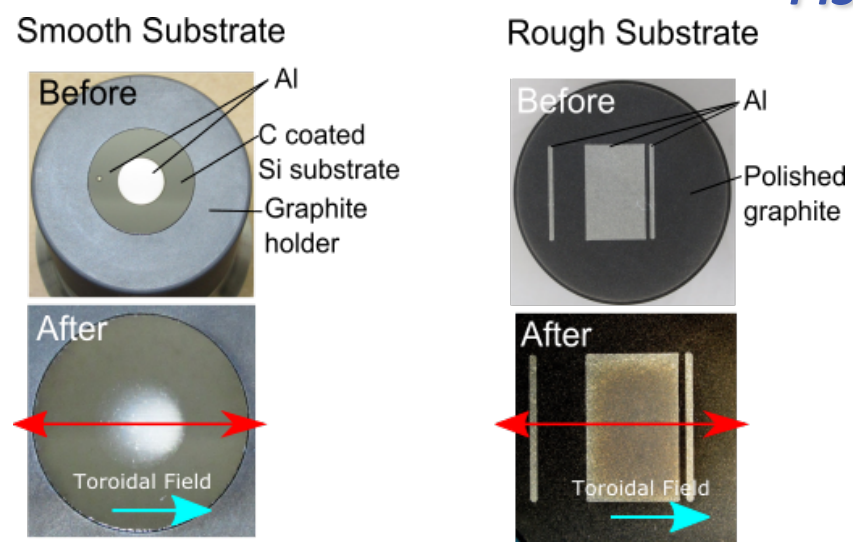


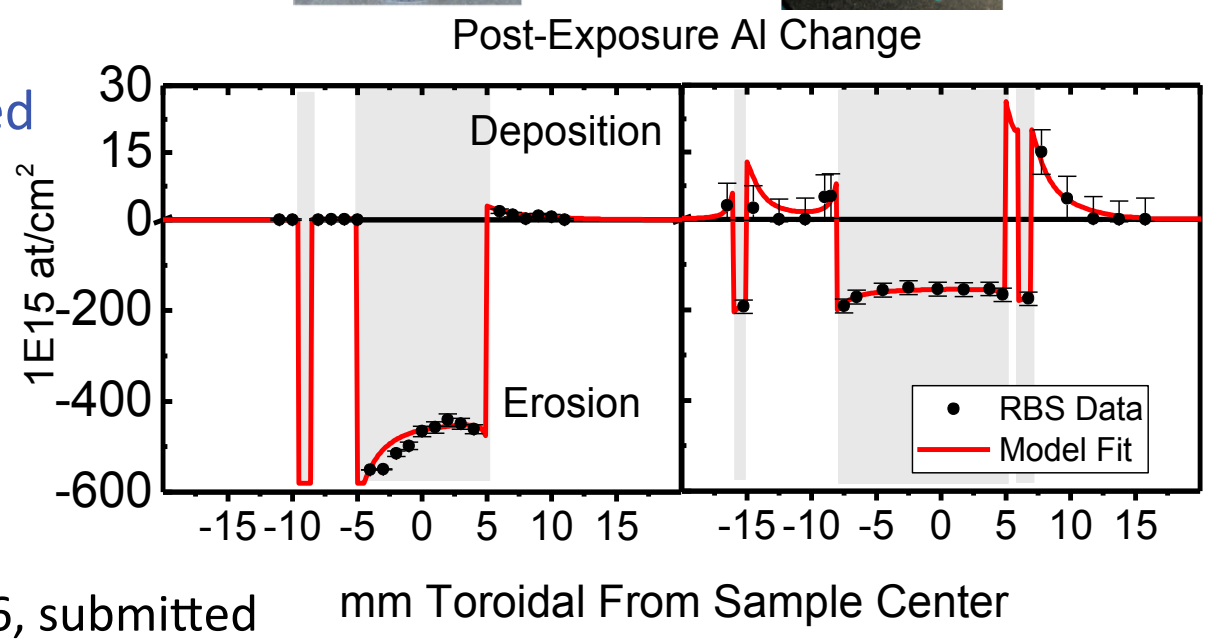
Gosselin, PhD 2016, submitted

Modeling Material Migration in DIII-D

PISCES

- Multi-step erosion/deposition process leads to rapid directional migration of eroded material.
- Substrate roughness increases deposit accumulation and decreases migration rate
- Material mixing and rough surface deposit accumulation modeled, reproducing observed results





DiMES
Divertor Material Evaluation System

Chrobak, PSI-2016, submitted

The PISCES Program participates in a variety of domestic and international collaborations

- ORNL
  - Steady-state Helicon source development for Proto-MPEX
  - Material property changes varying plasma flux to surfaces, fuzz properties
  - RF Antenna INSULATOR erosion due to long-term plasma exposure
  - W isotopic coatings for determining fuzz growth mechanisms
- DIII-D
  - DiMES materials exposures (pre-treated PISCES W samples, low-z erosion measurements)
  - Qualification test for metal ring campaign
- LANL
  - Ion Beam Materials Lab, High energy ion beam damage of W, nano-indentation

The PISCES Program participates in a variety of domestic and international collaborations

- US-EU Bilateral Agreement
  - Dr. D. Alegre (CIEMAT 1 yr. visit), He retention in Be
  - IPP Garching, Ion beam analysis of samples (including Be), Displacement damage studies
  - U. Helsinki, Be surface analysis measurements
- US-Japan technology exchanges
  - TEM analysis of samples (including Be)
- China
  - Advising in construction of PISCES-like facility w/ integrated ion beam, new PMI Center at Southwestern Inst of Physics (Chengdu)

Open questions

- Why the difference between ion beam, neutron irrad. thermal conductivity
  - Surface effect?
    - Try deeper ion beams (~10 MeV H/He damage to ~10 micron)
  - Fast particle energy spectrum effect?
  - Damage production rate?
    - Vary beam current & look for changes

High impact on divertor target performance – Need deep understanding of these results

Open questions (cont'd)

- Annealing of damage at high temperature shows large effect on retention, but…
  - Can simultaneous D/He implantation immobilize vacancies?
  - If so, what implantation rate needed to affect vacancy annihilation?
  - Will plasma-implanted D/He reduce/eliminate annealing effects?
  - Can we develop a validated predictive model for retention in damaged PMI surfaces?

Motivates simultaneous plasma/beam experiments

Open questions (cont'd)

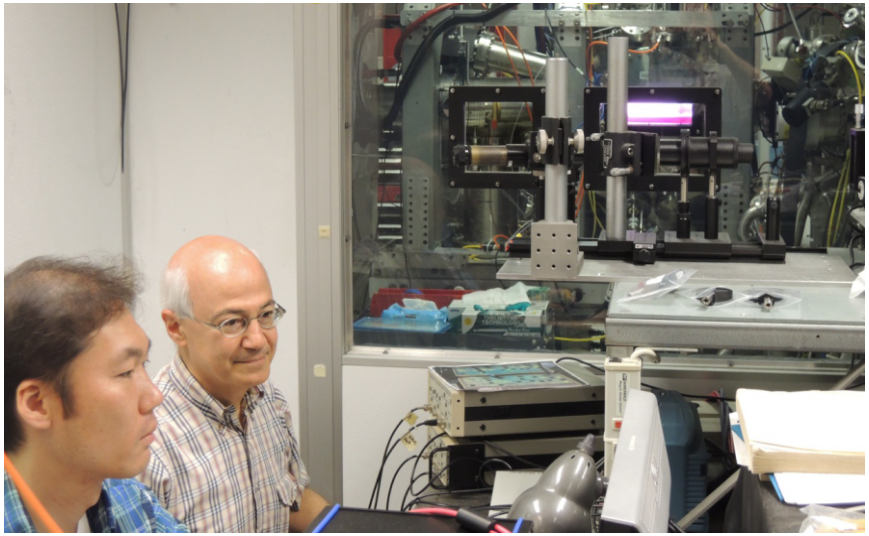
- How does retention probability vary with net plasma ion fluence & damage?
- Do He-nanobubbles form & inhibit D diffusion in damaged W exposed to mixed D/He plasmas?
- Does retention become low enough for TBR>1 & T inventory limits?
  - **Need higher fluence mixed D/He retention studies**
    - **<10 microns: >MeV H/He ion beams + high flux plasmas**
    - **>10 microns: neutron irradiation + high flux plasmas**
    - +Multi-scale (DFT/MD/Continuum) modeling

BACKUP MATERIAL

PISCES offers a unique platform to study the fundamental science of PMI

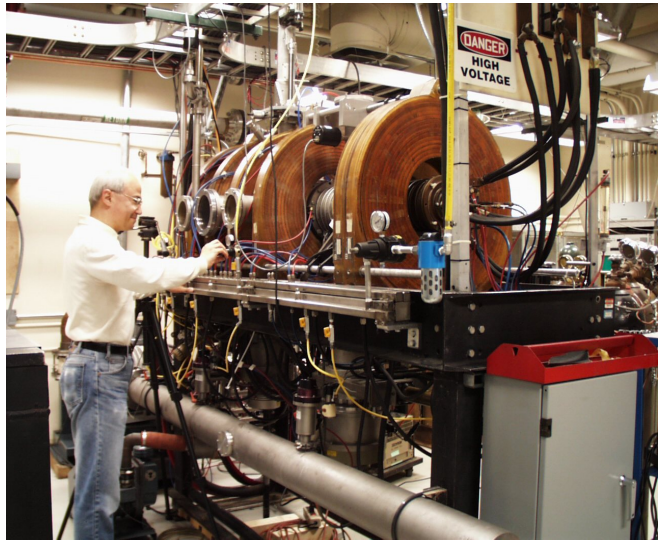
- In addition to being the most powerful, steady-state plasma source in the world, PISCES-B has several unique capabilities
  - Compatible with Be operations
  - In-vacuum surface analysis coupled to plasma chamber
  - Transient laser heating of surfaces during plasma exposure (fs to cw)
  - Controlled impurity seeding of the plasma
  - Witness plate collector for codeposition studies

	PISCES-B
Ion flux (cm^2s^{-1})	**10^{17}–10^{19}**
Ion energy (eV)	**20–300 (bias)**
T_e (eV)	3–40
n_e (cm^{-3})	**10^{12}–10^{13}**
Be Imp. fraction (%)	**Up to a few %**
Pulse length (s)	**Steady state**
PSI materials	C, W, Be
Plasma species	H, D, He

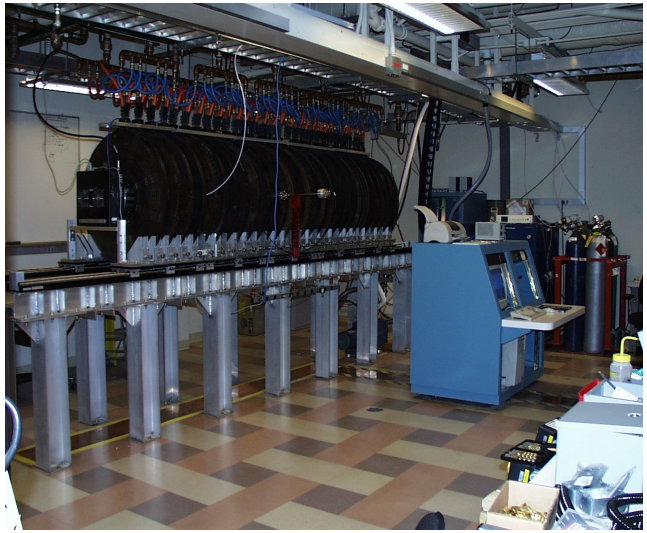


Auxiliary Facilities Support Research Goals

PISCES-A: PMI & Supporting Research



CSDX: RF Helicon Device For Edge & Divertor Physics



Surface Science Diagnostics

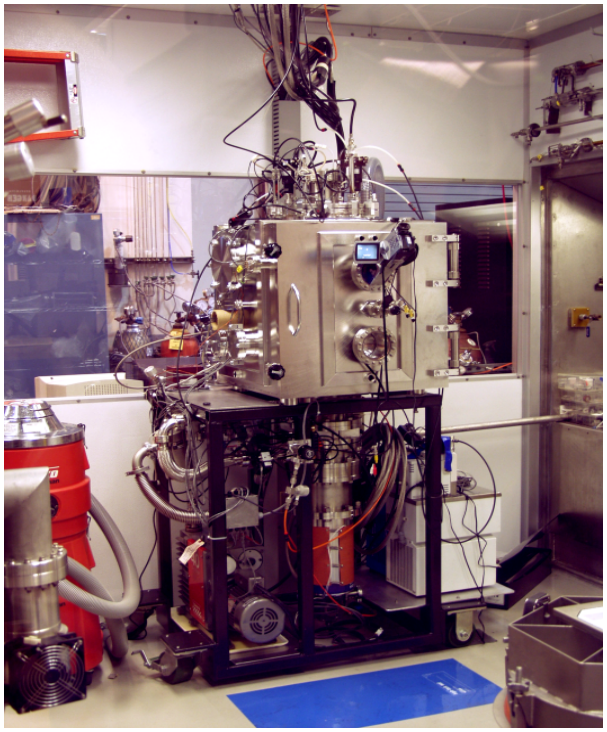
- *In-situ XPS, Auger, SIMS*
- *SEM with EDX/WDS*
- *Ex-situ SIMS, XPS, TDS*
- *Auxiliary Deposition Facilities*

Off-site Collaborations

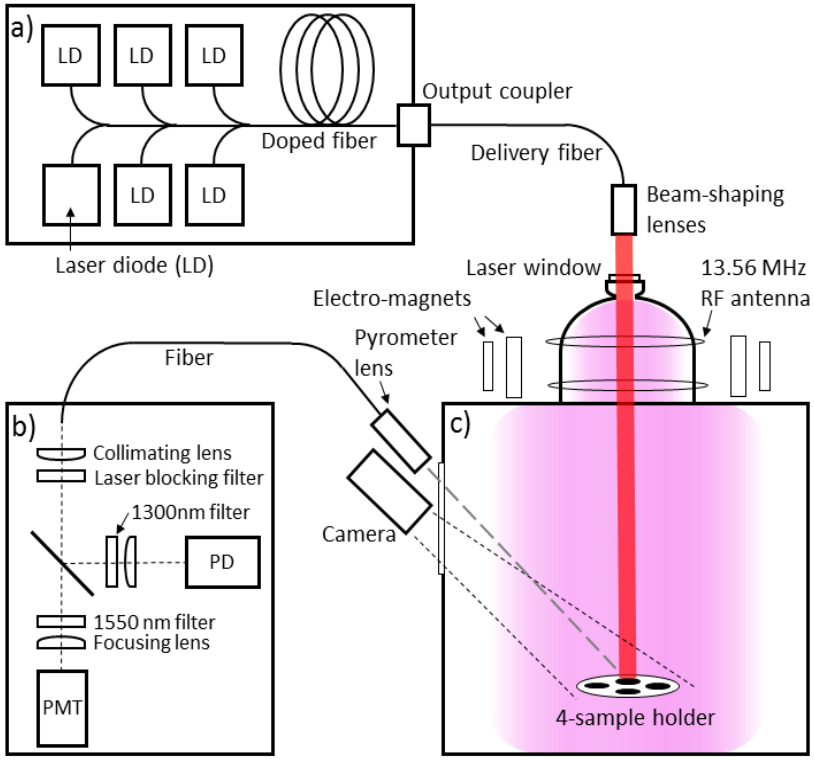
- *DIII-D, JET, EAST, HL-2A, AUG*
- *LANL: IBML w/ Dual-Ion Beam & Nano-lab Facilities*
- *SNL*
- *IPP-Garching PMI Group*

Auxiliary Facilities Support Research Goals

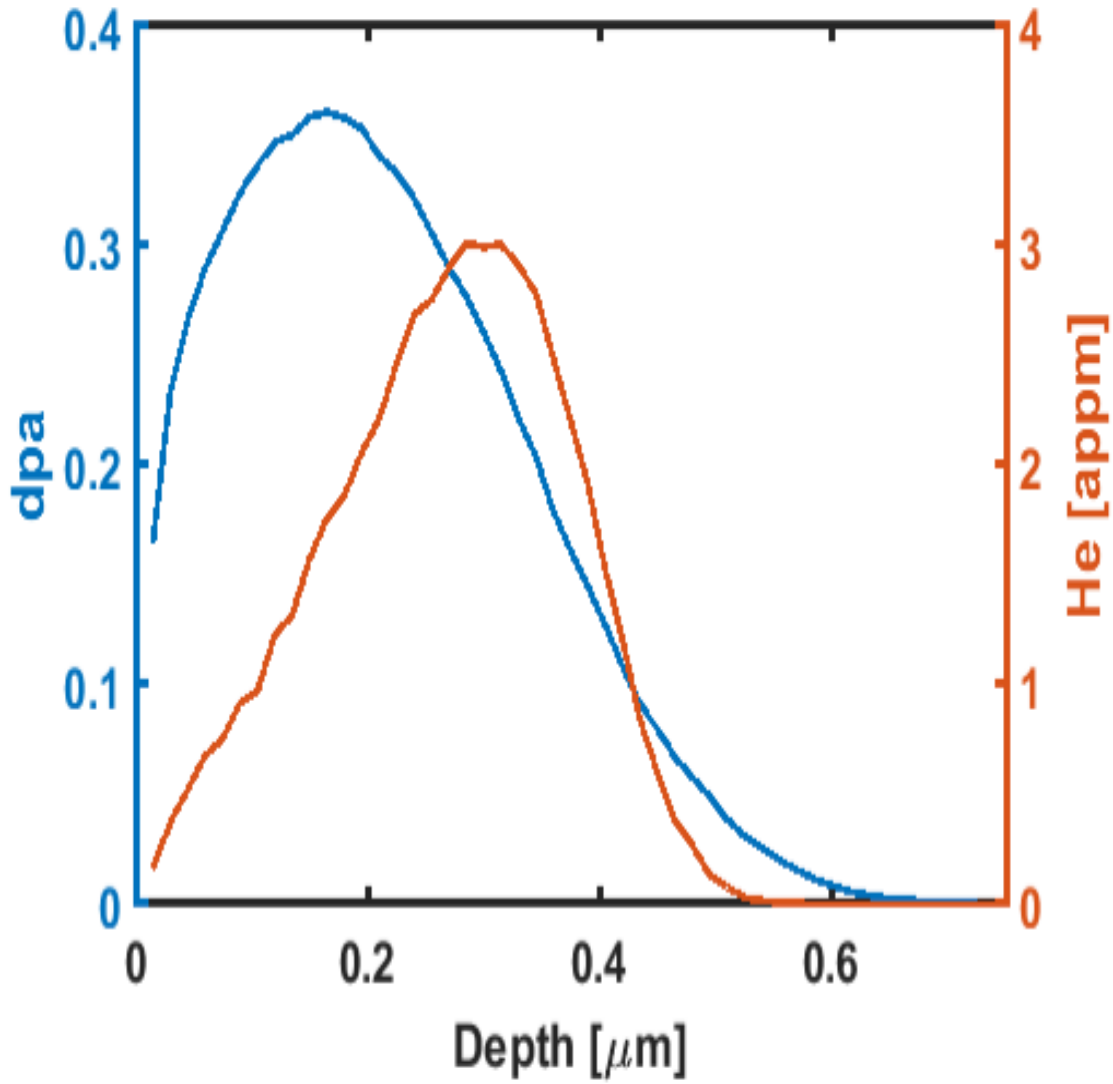
Magnetron Sputtering (including Be-capable)



Intermediate Flux RF Source w/ Pulsed Laser, In-situ plasma mass spec, DC & RF Biased Sample Holder

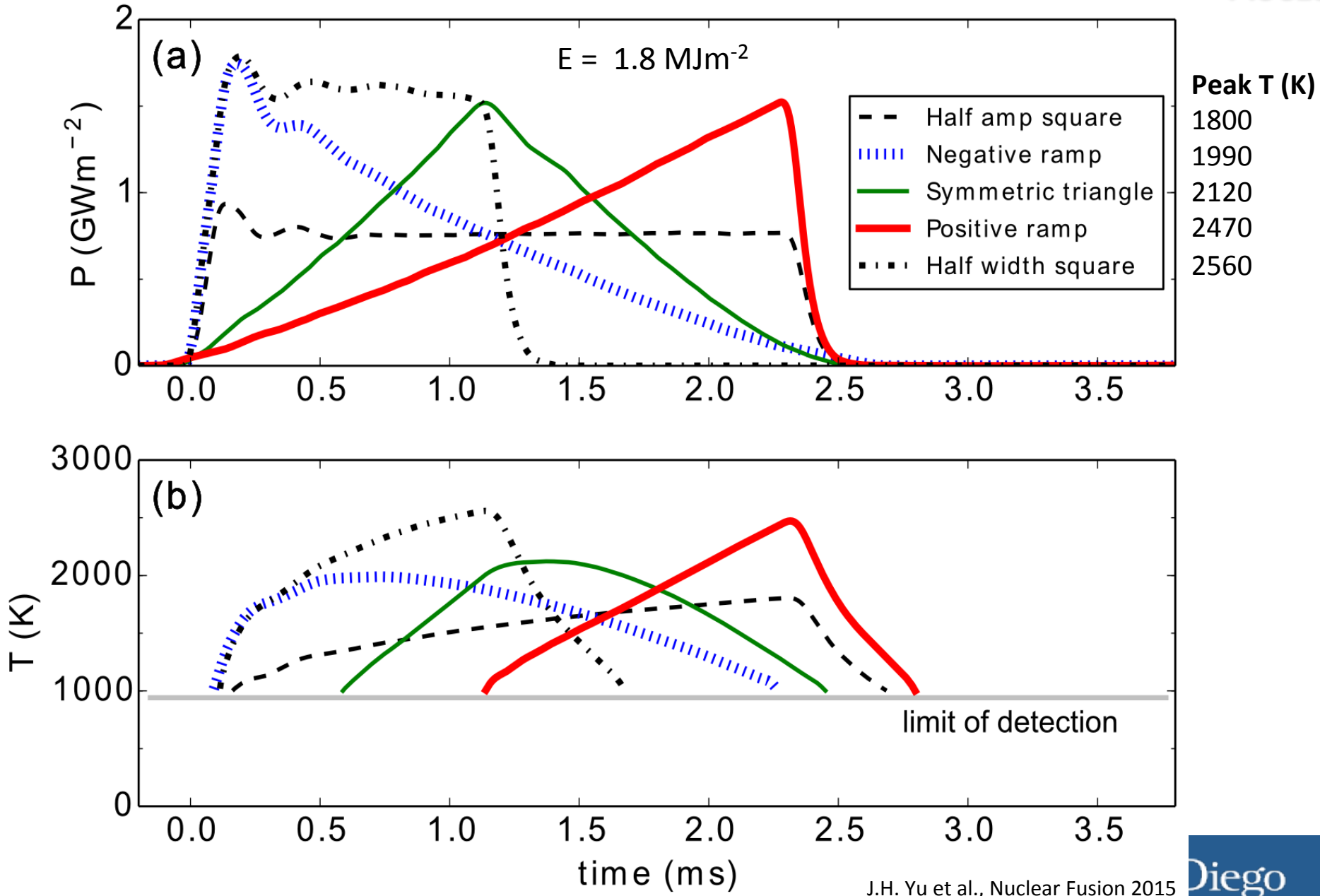


Backup Slide: Dual Beam Damage Profile



- Cu displacement damage (Blue)
- He ion range (Red)
- Peaks do not line up due to an error while performing Cu damage (Cu^{2+} used instead of Cu^{3+})

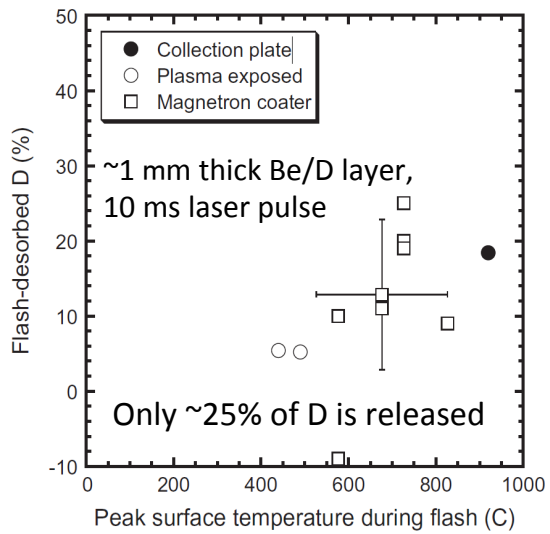
Peak surface temperature depends on pulse shape, even with same energy density and same pulse width



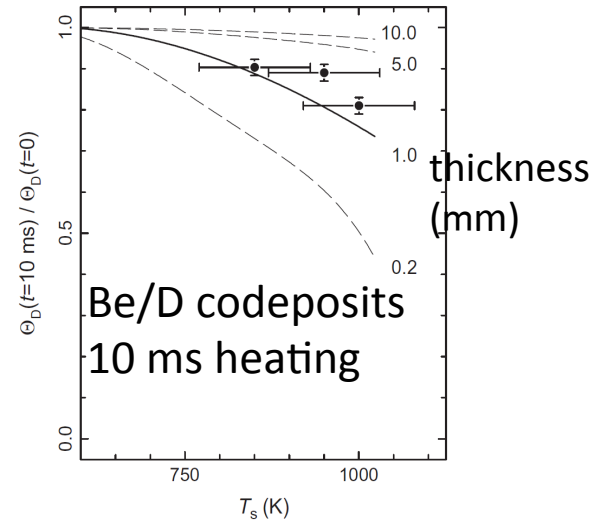
J.H. Yu et al., Nuclear Fusion 2015

D takes longer time and higher T to desorb from Be/D codeposits

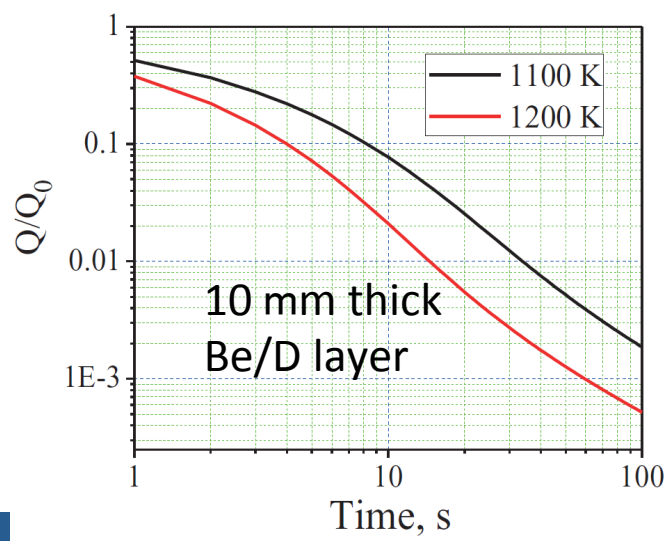
Laser heating, J.H. Yu et al., JNM 2013

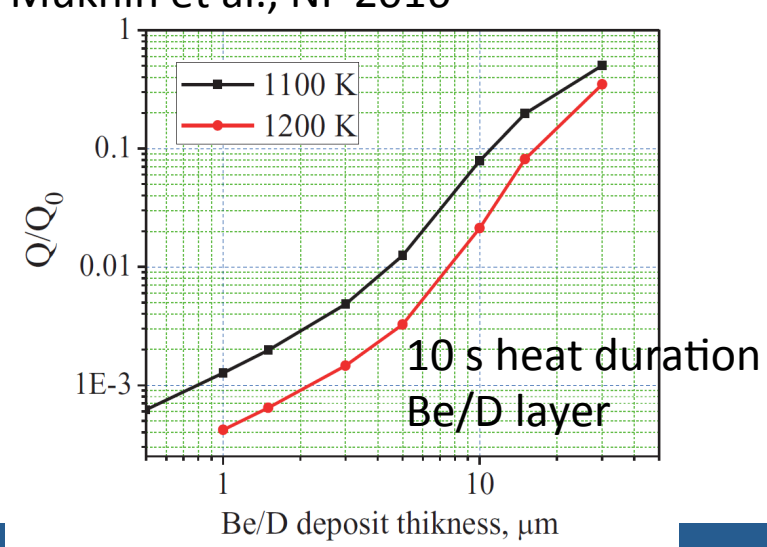


TMAP7 modeling, M.J. Baldwin, JNM 2013

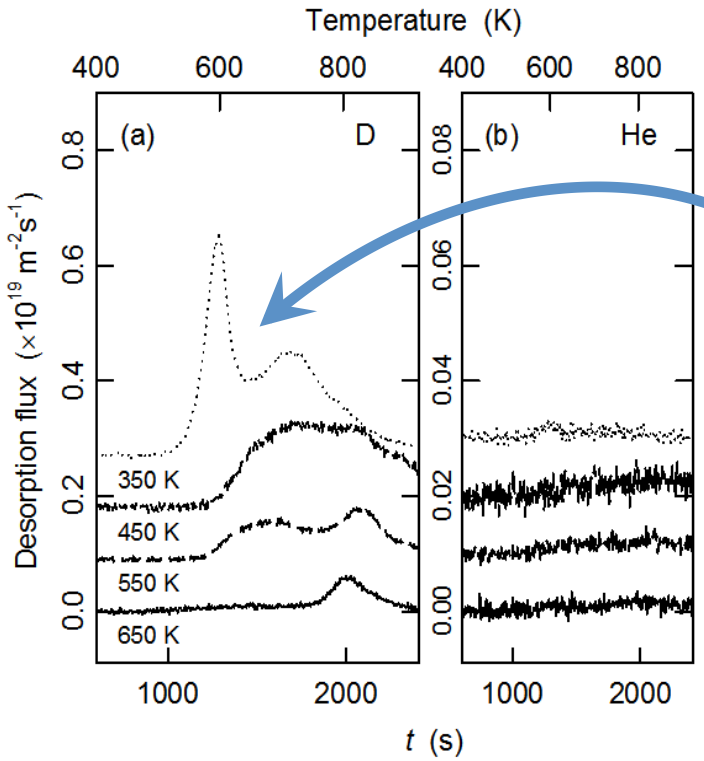


TMAP7 modeling, E.E. Mukhin et al., NF 2016

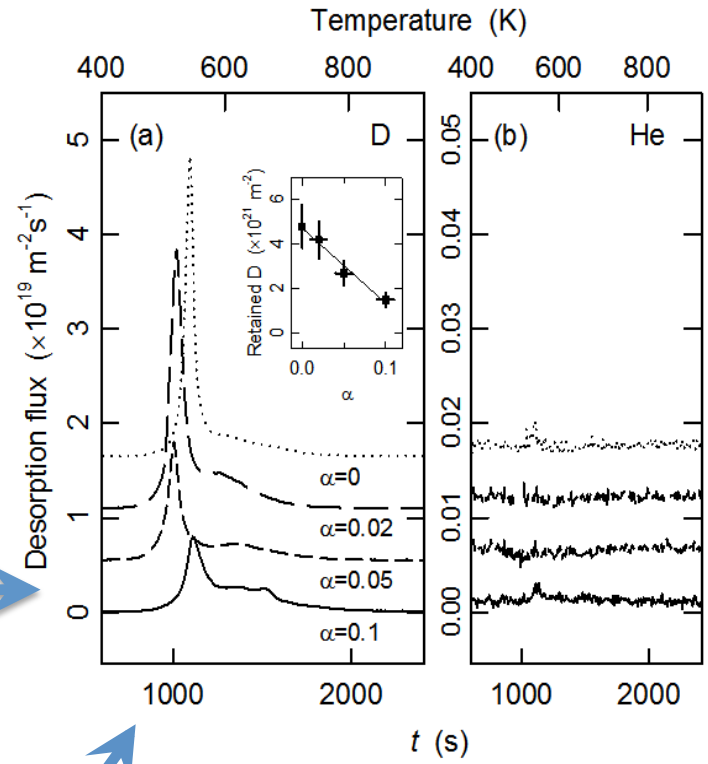




Similar D retention reduction observed in Be



- TDS data for Be exposed to D-He plasmas
- D traps : 550, 700, 800 K.
- Low/no He release < 923 K.
- 10% He (a= 0.1) affects 550 K D trap.

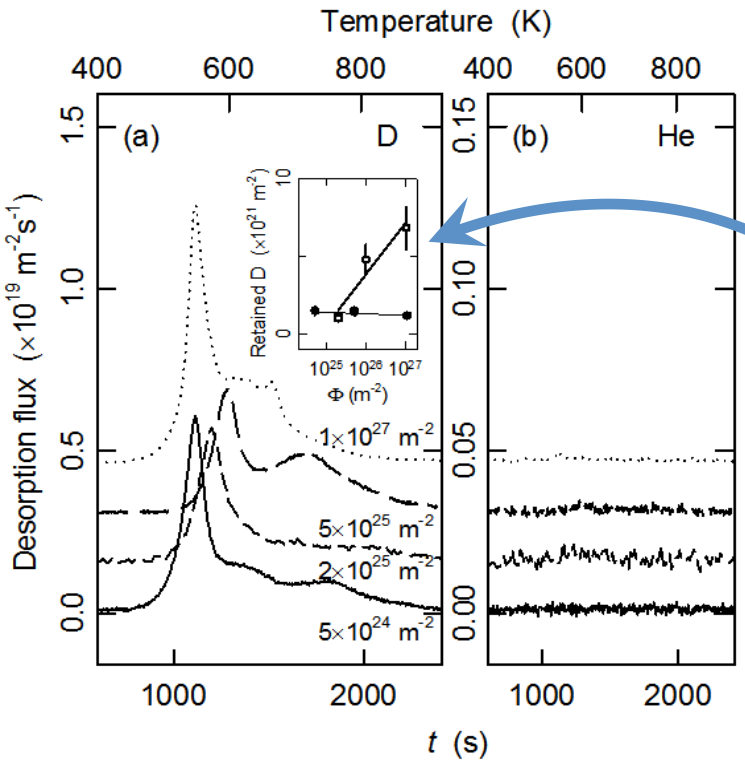


α	0.1	
T_{exp}	**330 – 650**	**(K)**
Φ	5×10^{25}	(m^{-2})
E_i	40	(eV)

α	**0.0 – 0.1**	
T_{exp}	330	(K)
Φ	1×10^{26}	(m^{-2})
E_i	40	(eV)

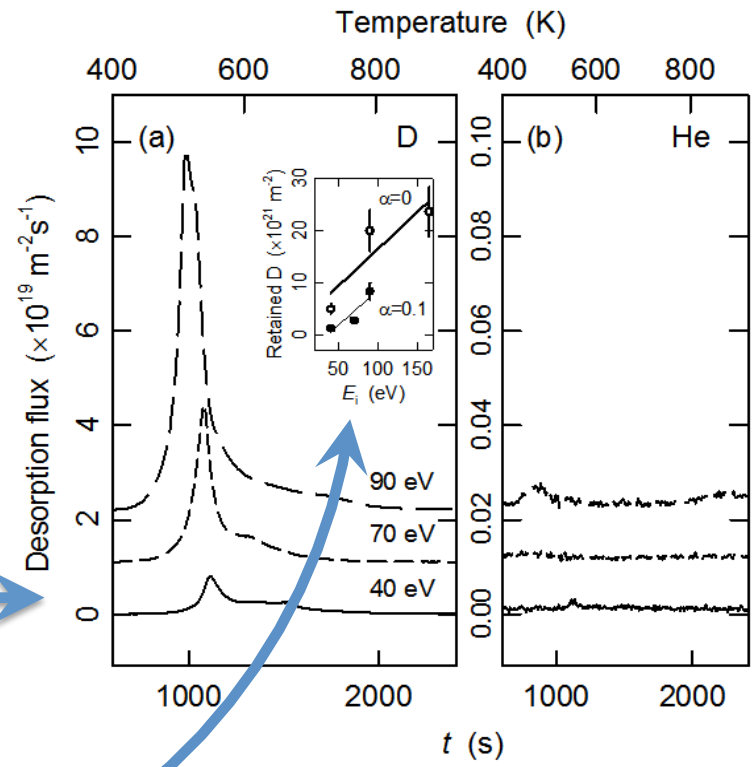
Similar effects observed in Be

350 K, 10 % He



α	0.1	
T_{exp}	**330 – 650**	**(K)**
Φ	5×10^{25}	(m^{-2})
E_i	40	(eV)

- Be exposed to D-0.1He plasma
- Fluence dependence altered.
- Low/no He release < 923 K.
- Ion energy dependence similar, but reduced in magnitude.

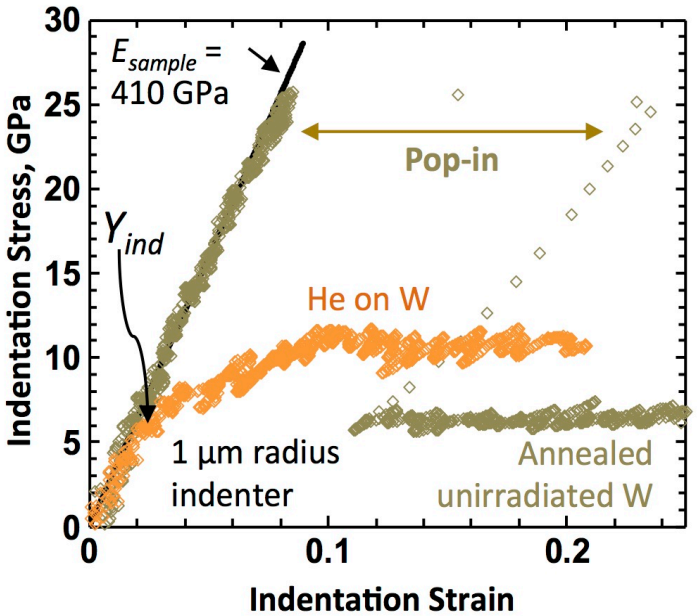


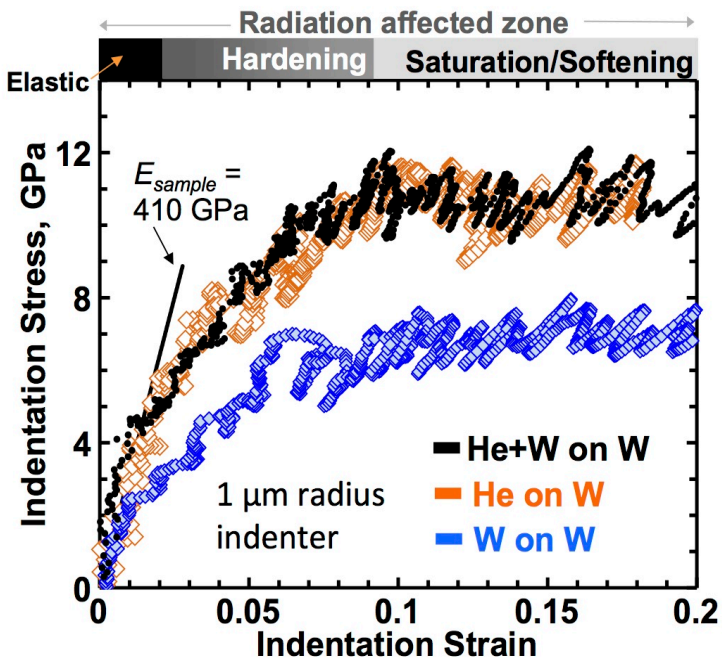
α	**0.0 – 0.1**	
T_{exp}	330	(K)
Φ	1×10^{26}	(m^{-2})
E_i	40	(eV)

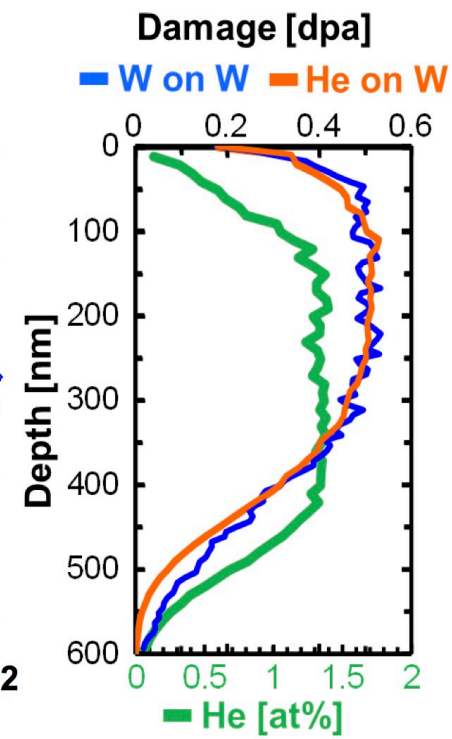
Comparison of D desorption from W and from Be/D codeposits

- TMAP7 modeling: of 10 mm thick Be codeposits predicts that ~2% of D is released after **10 ms at 1000 K**, while ~80% is released from W with same heating parameters.
- TMAP7 modeling of 10 mm thick Be codeposits predicts that ~50% of D is released after **1 s at 1100 K**, while >97% is released from W with same heating parameters.
- Why is less D released from Be codeposits compared to W?
    - Material properties (e.g., surface recombination)
    - Depth distribution of traps
    - Trap concentrations, possibly due to higher trap concentration in codeposits due to presence of BeD

Modulus unchanged; few-x increase in hardness with 0.5 dpa He damage

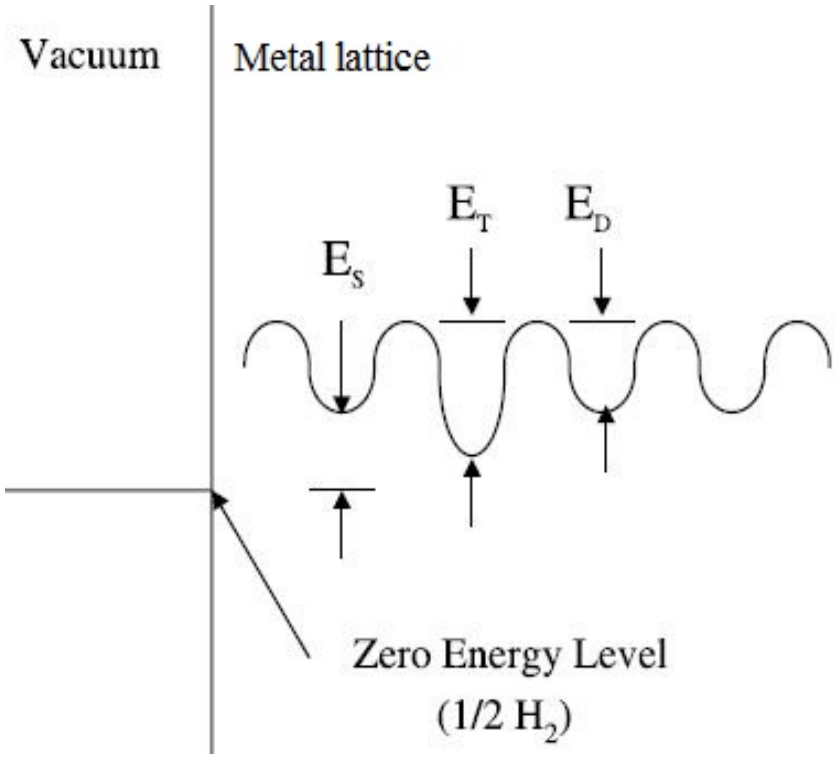






Diffusion Model

Calculating the concentration of trapped D in lattice defects after plasma exposure



Causey, J. Nucl. Mater. (2002)

- H isotopes can be trapped in defects
- Trapping energies taken from DFT models - only defect densities are free parameters

Rate processes: trap effects and diffusion b/w traps

Trapping rate:

$$\alpha_{t,i} = \frac{D}{\lambda^2}\left(\frac{C_{\text{defect}} - C_{t,i}}{N_{\text{W}}}\right)$$

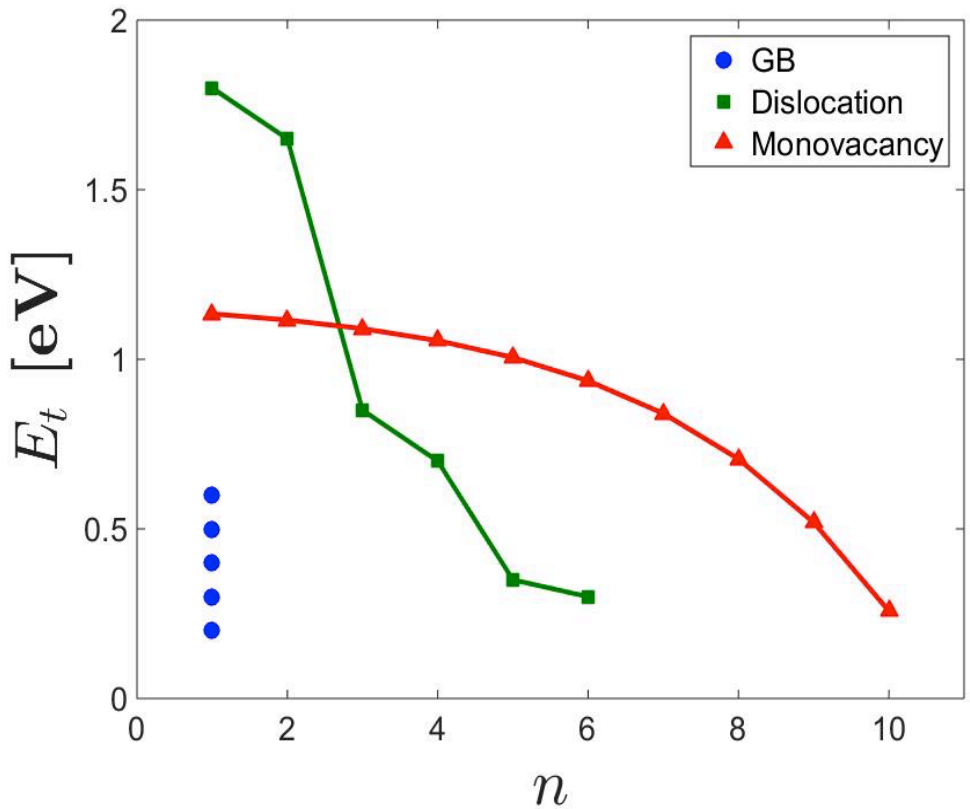
Release rate:

$$\alpha_{r,i} = \nu \exp\left(-E_{t,i}/T\right)$$

Diffusion rate:

$$\frac{D}{l_{\text{mfp}}^2} = D\left(C_{\text{defect}}\pi\lambda^2\right)^2$$

Trapping energies from DFT



- Release rate completely defined
- GB, dislocation and monovacancy defect densities are the only free parameters

GB: Zhou, et al., Nucl. Fusion (2010)
Dis: Xiao, et al., J. Nucl. Mater. (2012)
Vac: Liu, et al., Phys. Rev. B, (2009)

Rate processes: trap effects and diffusion b/w traps

Trapping rate:

$$\alpha_{t,i} = \alpha_{t,i}^{0}\left(1 - \frac{C_{t,i}}{C_{\text{defect}}}\right)$$

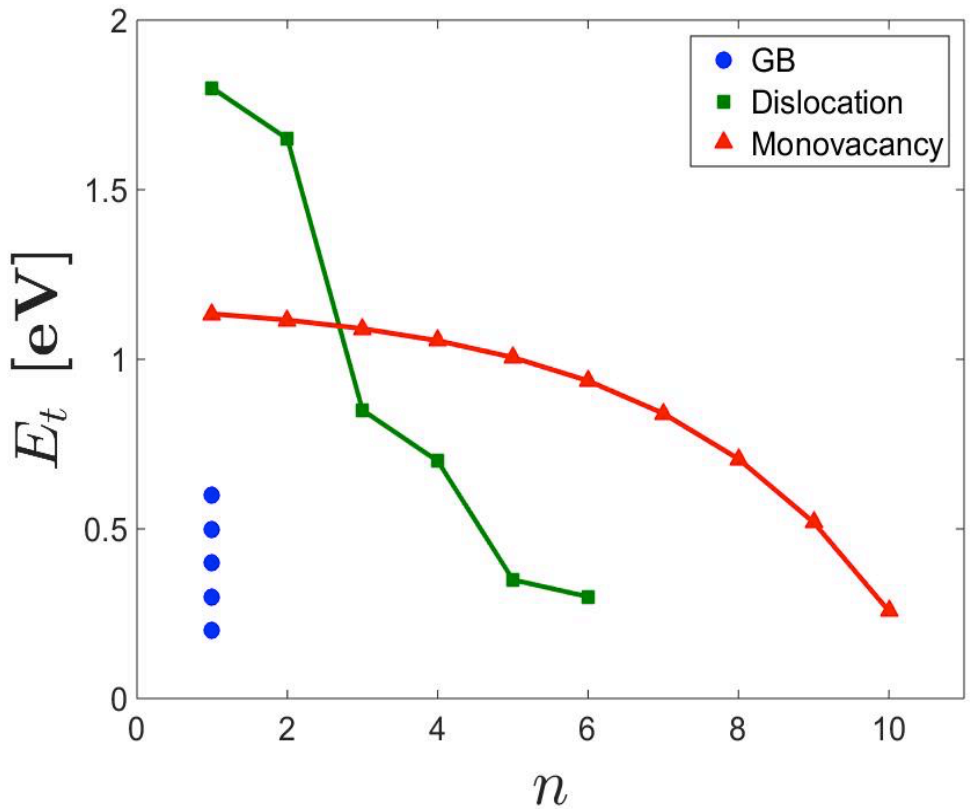
Release rate:

$$\alpha_{r,i} = \nu \exp\left(-E_{t,i}/T\right)$$

Diffusion rate:

$$\frac{D}{l_{\text{mfp}}^{2}} = D\left(C_{\text{defect}}\pi\lambda^{2}\right)^{2}$$

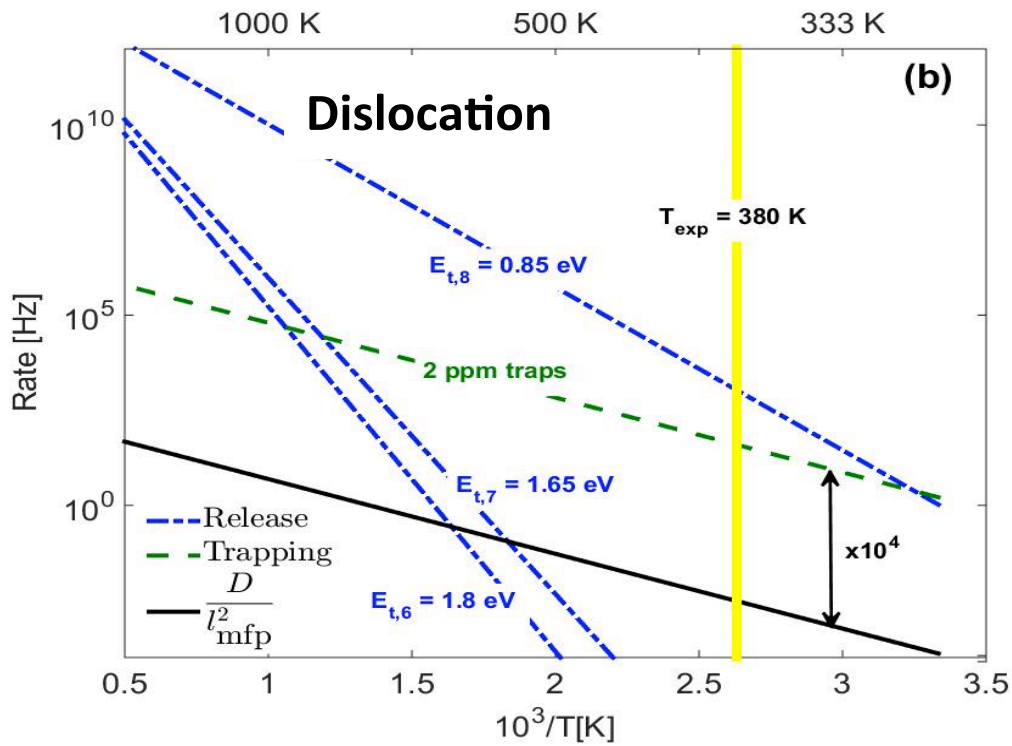
Trapping energies from DFT



- Release rate completely defined
- GB, dislocation and monovacancy defect densities are the only free parameters

GB: Zhou, et al., Nucl. Fusion (2010)
Dis: Xiao, et al., J. Nucl. Mater. (2012)
Vac: Liu, et al., Phys. Rev. B, (2009)

Rate limiting factors suggest equilibrium condition



Barton, et al., J. Nucl. Mater. (2015)
Barton, et al., Nucl. Fusion (submitted 2016)

$$(\alpha_{t,i} \sim \alpha_{r,i}) \gg \frac{D}{l^2_{\mathrm{mfp}}} \quad \& \quad \alpha_{t,i} \gg \frac{D}{l^2_{\mathrm{mfp}}} \gg \alpha_{r,i} \quad \Rightarrow \quad \alpha_{t,i} C_s = \alpha_{r,i} C_{t,i}$$

Local equilibrium condition (LEC): slowly diffusing concentration of solute atoms that achieve an equilibrium value with the trapped concentrations before diffusing further

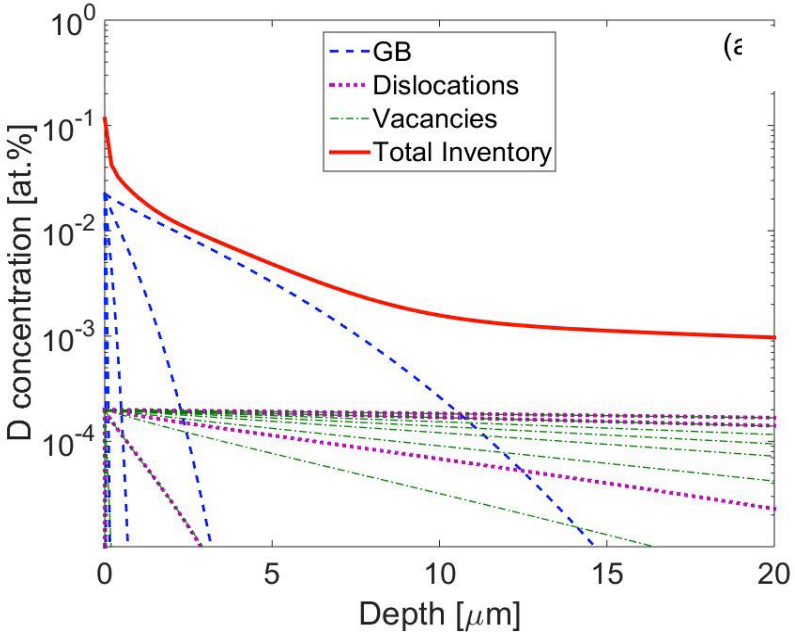
Motivated by this LEC we propose a diffusion equation for the trapped concentration

$$\begin{cases} \dfrac{\partial C_{t,i}}{\partial t} = D\dfrac{\partial^2 C_{t,i}}{\partial x^2} - \dfrac{\partial C_s}{\partial t} \\ \alpha_{t,i} C_s = \alpha_{r,i} C_{t,i} \end{cases}$$

Substituting for C_s and collecting terms

$$\frac{\partial C_{t,i}}{\partial t} = D_{t,i}\frac{\partial^2 C_{t,i}}{\partial x^2}$$

$$D_{t,i} = \frac{D}{1 + \dfrac{\alpha_{r,i}/\alpha^o_{t,i}}{(1 - C_{t,i}/C_{\text{defect}})^2}}$$



The total trapped D

$$C^{\text{tot}}(x, t_{\text{exp}}) = \sum_i C_{t,i}(x, t_{\text{exp}})$$

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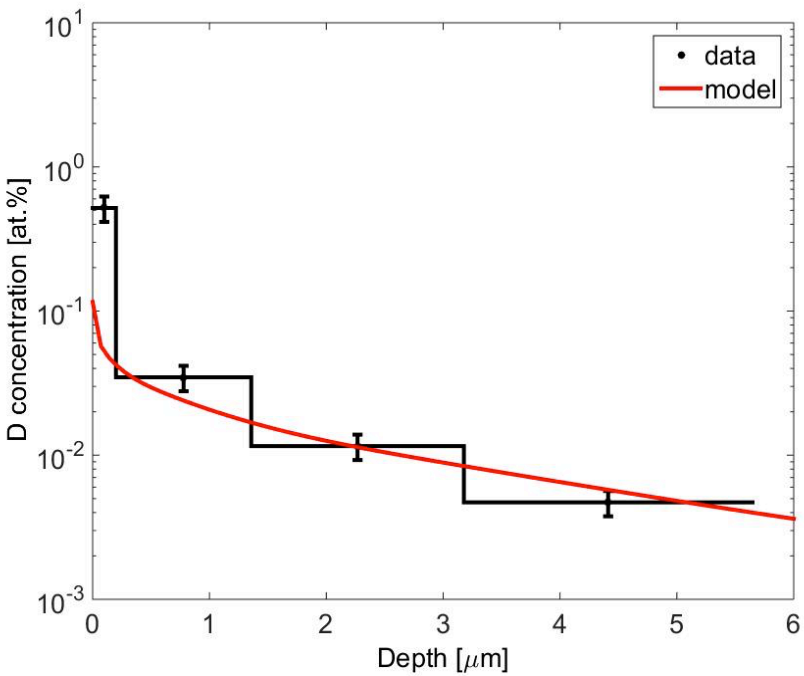

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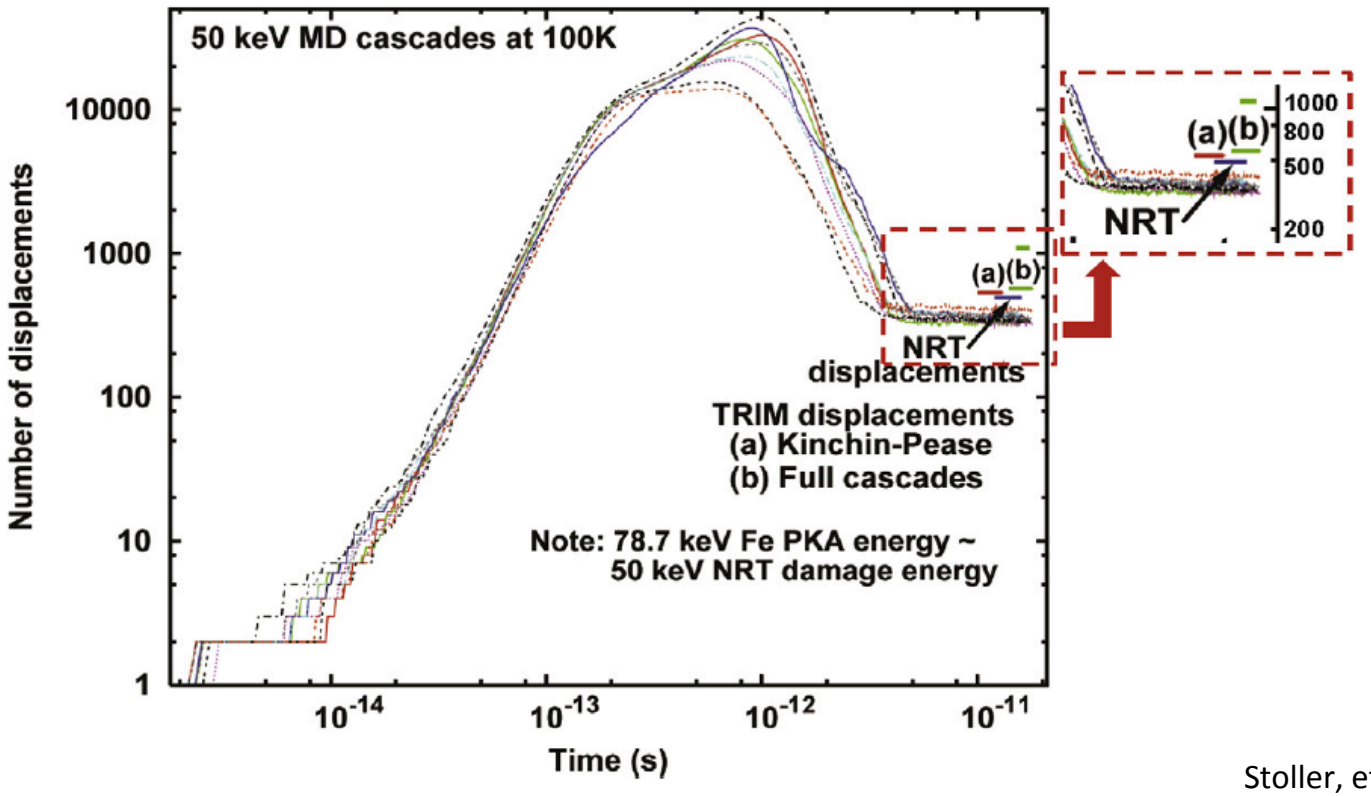
$$C^{\text{tot}}(x, t_{\text{exp}}) = \sum_i C_{t,i}(x, t_{\text{exp}})$$

SRIM over-estimates vacancy density

- Temperature affects not taken into account
- W interstitials are known to migrate at T>27 K [Averback, et al. (1997)]

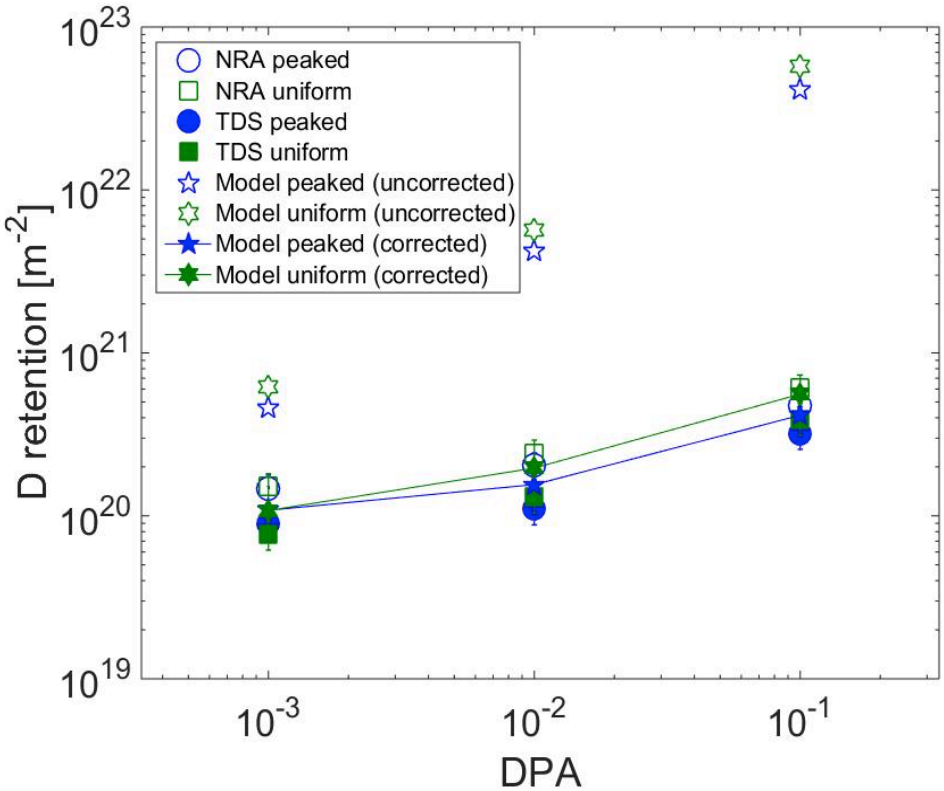
Comparison of MD vs SRIM vacancy densities of self-damaged Fe

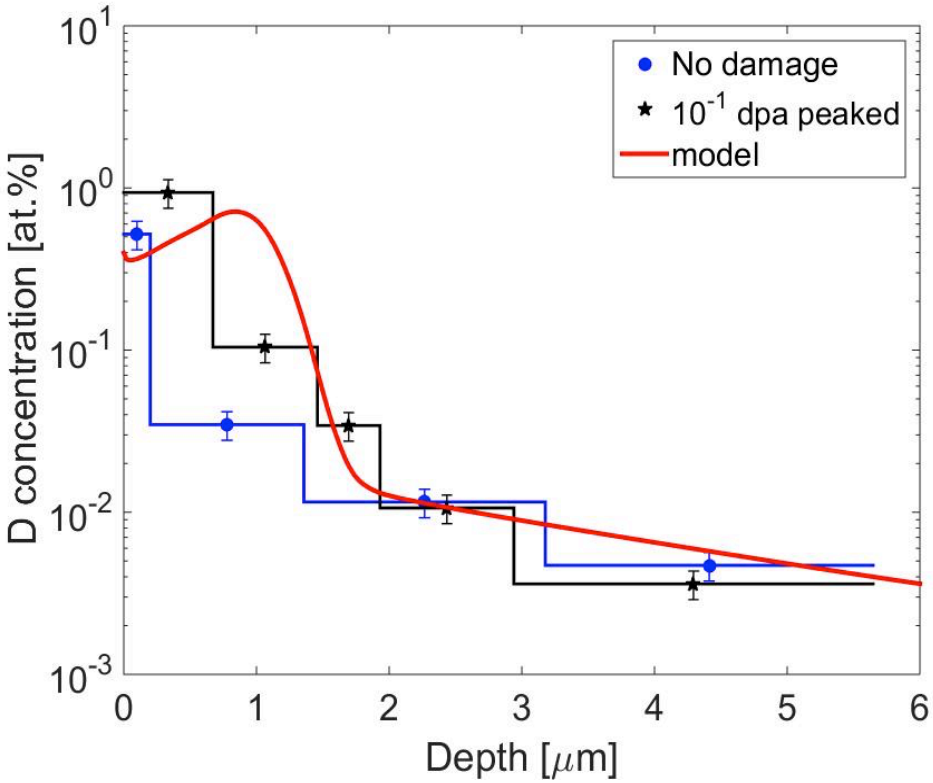


Stoller, et al., NIM B (2013)

Model ion damage by modifying the monovacancy trap density: $C_{defect}(x)$ from SRIM

- C_{defect} for intrinsic defects are now fixed
- Only monovacancies produced with damage at T< 573 K [1-2]
- For vacancies: $C_{defect}(x) = C_{defect,intrinsic} + C_{defect,SRIM}(x) / q$; $q>1$





[1] Stoller, in "Comprehensive Nuclear Materials" (2012) [2] Shimada, et al., Nucl. Fusion (2015)