Scientific Challenges in the Fusion Plasma-Material Interface

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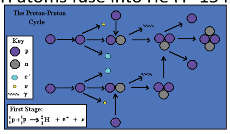
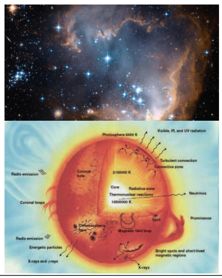
Astro-fusion against terrestrial fusion?

Fusion in stars

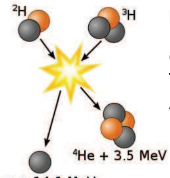
- Process in the core of our Sun and stars: H atoms fuse into He (T=15 mil)





the energy release rate in sun is only 276 μW/cm³
Impractical for terrestrial conditions

Fusion on earth (Controlled fusion!)



d-t fusion (more efficient)
T=150 mil K
Alpha-particles and neutrons carry most of the energy

Layout:

1. QUESTIONS:

Why is PMI of high importance for the controlled nuclear fusion?
Why is it so difficult problem?
How to build an effective scientific approach to study PMI, recognizing its multiscale character?
How to validate theory with the plasma-facing surface experiments?
How could be PMI processes in giga machines compared with atomistic results?
What is the role of quantum mechanics and role of chemistry?
What are the bounds of uncretainty of the PMI data?
How to build an integrated theoretical-experimental approach?
How to build an intergated and self-consistent PMI-plasma approach?
Quality assurance?

2. LITHIUM?

1. TUNGSTEN?

Challenges with tungsten in fusion

Neutron inflicted defects

- 14 MeV Neutrons? Energetic particles?

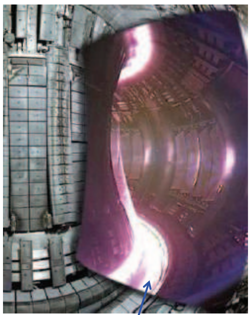
High Temperatures!

For realistic energy conversion (DEMO)
need a hot surfaces > 600C
Carnot thermodynamical process
of high efficiency is needed

On the other hand:
ITER will work at low T's (400K)
Most of the experiments done at room temperature (300K)

Tungsten in Future Fusion Devices

- Tungsten (W) is the **only candidate for plasma-facing material** in next-generation magnetic fusion devices due to several favorable properties:
  - High melting point
  - High thermal conductivity
  - High sputtering energy threshold
  - Low sputter yield
- However, it has recently been discovered that **interactions of He ions** produced by D-T fusion reactions with W surfaces can **cause morphological changes** even at low impact energies (~100 eV), including formation of "nano-fuzz"
- **Why is nano-fuzz undesirable** for plasma-facing materials?
  - Reduces thermal conductivity of material
  - Potential source of deleterious high-Z dust impurity in fusion plasma
  - Possible increased retention of tritium in material



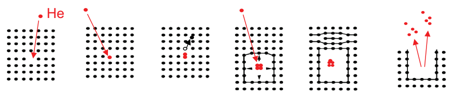
Tungsten divertor tiles

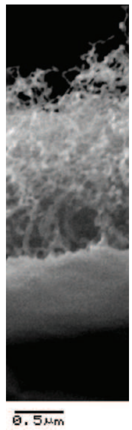
What is Nano-fuzz?

High-flux He-ion irradiation of hot tungsten surfaces can induce significant surface morphology changes:

- Beyond a critical ion flux, W exhibits **chaotic tens-of-nm-diameter tendril growth** that is independent of surface grain orientation. But there is still **no coherent picture of why flux threshold exists** and what its defining factors are
- For He-ion impact energies **below the displacement damage threshold**, growth of nanostructures due to He trapping at **intrinsic or extrinsic defect sites** with subsequent dynamics of near-surface cluster nucleation, bubble formation, coalescence, growth, and ultimately bursting, although **exact mechanisms and processes still not understood**
- The effects of extrinsic trapping sites due to **impurities** and **radiation damage** are presently not known

A fundamental science understanding is needed to provide a **rational basis** for development of fuzz-resistant materials.

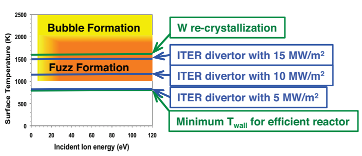




Nano-fuzz will likely form under He bombardment in future fusion reactors

Growth conditions for W fuzz are well-defined from experiments on linear plasma devices
G.M. Wright, 54th APS-DPP, Providence, 2012

Nano-fuzz growth condition	ITER or Reactor condition	Nano-fuzz growth?
Bare W or Mo	Bare W in net erosion regions and entire first wall	☑
1000 K < surface temp < 2000 K	ITER divertor, 5 MW/m^2 ➔ 830 K, 15 MW/m^2 ➔ 1500 K Reactor W will operate 800 K – 1600 K	☑
He-ion (E > 20 eV) flux > 10^{20} m^{-2} s^{-1}	ITER ion fluxes of ~10^{24} m^{-2}s^{-1}, only 1 % He content needed for maximum fuzz growth rate	☑



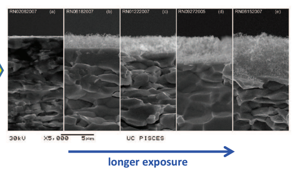
S. Kajita *et al.*, Nucl. Fusion **49**, 095005 (2009)

M.J. Baldwin *et al.*,
J. Nucl. Mater. **390-391**,886 (2009)

Previous Nano-fuzz Research

- First investigations of nano-fuzz production on hot tungsten surfaces by He-ion exposure were performed with linear plasma devices – NAGDIS, PILOT-PSI, and PISCES-B – with ion energies below 200 eV (but broad energy distribution):
  - Nano-fuzz formation observed for fluxes > 10^{20} m^{-2} s^{-1} and T > 1100 K
  - Nano-fuzz thickness grew as square-root of exposure time, interpreted as diffusive mechanism

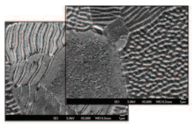
Plasma impact, questionable impurity content
Poor vacuum
Unknown surface condition
Only normal incidence
Max energies < ~200 eV



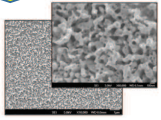
Baldwin/Doerner (2008)

Mono-energetic ions,
Ultra-high vacuum,
Well-characterized surface and ion beam
Large range of incidence angles
Energies up to 250 kVxq

- Investigation at MIRF on rolled W sheet stock performed with **mono-energetic** He-ion beams down to 80 eV:
  - Nano-fuzz formation observed for fluxes > 1.5 x 10^{20} m^{-2} s^{-1} and T > 1100 K



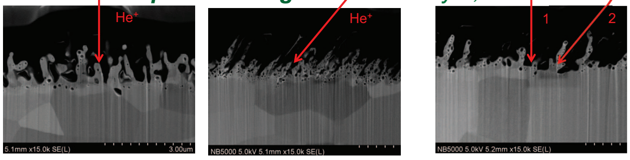
below flux threshold



above flux threshold

Bannister, Meyer, ORNL

+Plasma synergy: ***Incidence angle dependence and dual exposure He impact on tungsten*** *F.W. Meyer, 2013*



normal incidence | *43⁰ away from normal* | *normal incidence exp. (1) followed by 43⁰ exp. (2)*

F.W. Meyer, 2013

- ***The fuzz growth remembers the incidence angle***
  - ***So not totally random***
- ***Reduced tendril density after dual exposure***
  - ***Due to enhanced sputtering?***

10 keV Incident energy

Incidence angle exp studies only possible using ion beam approach (currently)!

Mass loss would have significant implications for W-based magnetic fusion devices (e.g. during disruptions, when incidence angle and energy can change)

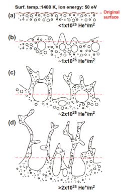
NEW!

At sub-100 eV He impact energy Fuzz-growth not following the impact direction! (Meyer, Bannister, 2014)
This research is ongoing at ORNL-MIRF!

Nano-fuzz Formation Still Not Understood

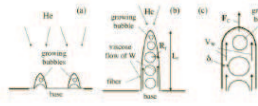
A number of explanations proposed:

Pinhole formation
Kajita et al. , JNM 2011



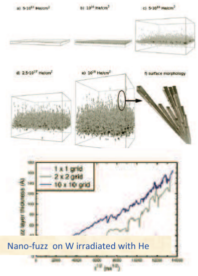
Qualitative only

"Visco-elastic" growth model
Krashenninikov, Phys. Script. 2011



Viscous W flow gives square-root of fluence dependence

MD/OKMC simulation
(Lasa et al., EPL 2014)



~~Surface roughness causes~~ √fluence dependence
Wrong flux ~~dependence~~

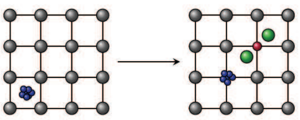
Need nano-fuzz measurements performed under well-characterized and well-defined conditions

Bannister, Meyer, 2014)

Key MD observations of early stage He bubble evolution

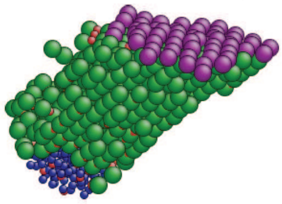
- **Helium insoluble but highly mobile and can self-trap (at high implantation rates) due to strong He-W repulsion to form highly mobile, strongly bound helium clusters**

B. Wirth, 2014



"trap mutation" processes

Occurs when 6–9 helium atoms coalesce, depending on temperature, after which bubble grows by absorbing smaller clusters.



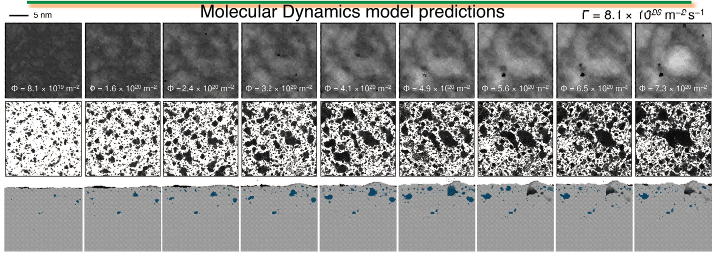
"loop-punching" processes

Movie available with F. Sefta, *et al. Nucl. Fusion* **53**: 073015 (2013)

- **Significant surface evolution through tungsten adatom formation, driven by trap mutation and loop-punching as tungsten interstitials rapidly diffuse to surface**
- ***As bubbles continue to grow at very high pressure, eventually rupture***

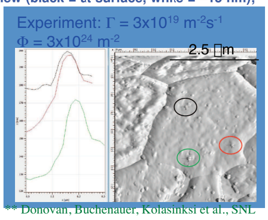
Tungsten surface response to low-energy He exposure

Molecular Dynamics model predictions



High-flux simulations showing surface growth and helium accumulation below a W(100) surface. Top: View of surface (white = +1.5 nm, black = −2 nm); Middle: helium atoms, top view (black = at surface, white = −15 nm); Bottom: cross-section.

- MD* of 100 eV He implanted into W reveals formation and growth of over-pressurized, sub-surface He bubbles thru self-trapping, trap mutation, loop punching and bubble bursting that evolve tungsten surface (hillocks & craters)
  → Qualitatively consistent with experiments** of W surface evolution following 60 eV He on tungsten
  → Quantitative comparison requires evaluation of rate & scale effects (Γ:MD 10^{26} vs expt 10^{19}; Φ: 10^{20} vs 10^{24})



* Hammond & Wirth, UTK/ORNL

** Donovan, Buchenauer, Kolasinksi et al., SNL

Neutron-caused defects simulated by effects of W self-atom (ion in exp.) damage

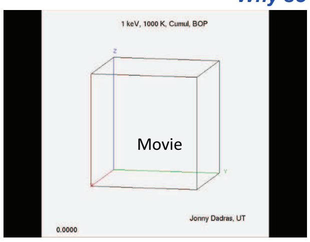
One way to study impact of 14 MeV neutrons and other light energetic particles

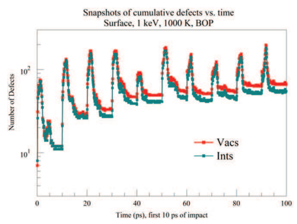
$$\frac{4M_1M_2}{(M_1+M_2)^2}E_{k0}$$

Exp::

- Virgin W has very low density of intrinsic defect sites at which to trap He
- 30 keV W ion exposure creates extrinsic near-surface defects that should facilitate He trapping during subsequent He ion exposures, perhaps even amorphize surface, and/or accelerate fuzz growth, but effect is small

Why so small effects?



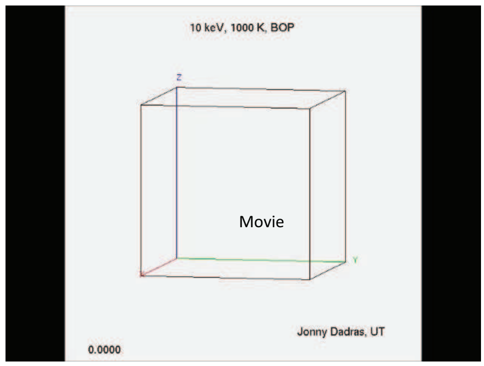


Strong recombination of Frenkel pairs

Evolution of Defects in a Tungsten Surface by Cumulative Bombardment with Self-Atoms: **Classical MD is here a good tool** !!! We choose LAMMPS and BOP

Krstic

10 keV W



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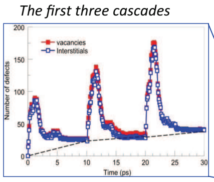
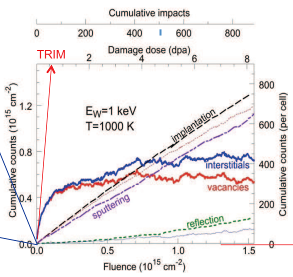
MD simulation of self-atom damage 1 keV

The first three cascades





Experimental W Self-ion fluence

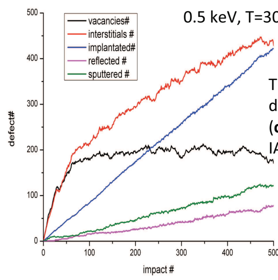
$10^{16}/cm^2$

Molecular dynamics results of damage accumulation for consecutive W impacts:
- *Unlike TRIM, accumulated damage is not linear with dose (# of impacts)*
- *In fact, accumulated damage saturates at much smaller doses than applied in expt.*
- *Evidence for spontaneous recombination of Frenkel pairs inside critical distance*

Recent experiments on deuterium retention in pre-damaged W by self-ions show saturation about 1 dpa!!!

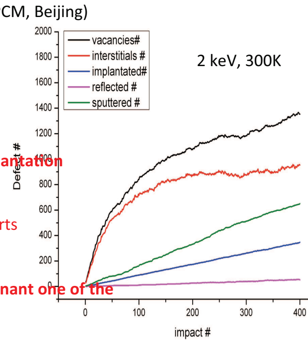
Krstic

0.5 keV, T=300K



The calculations of self-damage in tungsten done in range 250 eV -10 keV
(collaboration with Yong Wu, IAPCM, Fu Yong Zhao (2014) IAPCM, Beijing)

2 keV, 300K



- For impact energies < 2 keV implantation dominates over sputtering:
  Interstitials dominates vacancies
- At higher energies the trend inverts

At large fluences:
- The dominant defect linearly Increases with increase of the dominant one of the Implanted and sputtered;
- Sub-dominant defects saturates into a constant

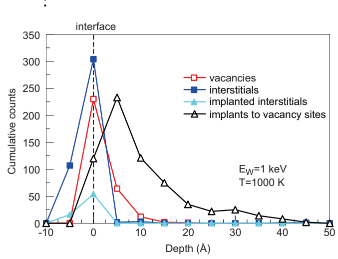
E(keV)	Vacancies			Interstitials			Sputt	Impl	Impl2	Refl
	A	B	C	A	B	C	D	E	F	G
0.25	181.37± 0.86	33.87 ±0.98	-0.163 ±0.001	*	*	0.56	0	0.88	0.16 ±0.001	
0.5	211.46 ±0.79	21.53 ±0.63	0	*	*	-0.10	0.25	0.85	0.10	0.14
0.75	361.40 ±1.40	55.89 ±1.00	0	*	*	-0.09	0.42	0.82	0.09	
1	410.33 ±1.20	42.15 ±0.67	0	*	*	-0.09	0.68	0.87	0.09	
2	*	*	1.01	1057.13 ±3.05	49.09 ±0.63	0	1.68 ±0.002	0.87	0.05	0.13
4	*	*	1.81	1268.91 ±5.10	49.45 ±0.88	0	2.23 ±0.003	0.87	0.03	0.13
6	*	*	2.06	3146.24 ±13.50	128.91 ±1.46	0	2.38 ±0.003	0.92	0.04	0.08
8	*	*	2.91	3333.16 ±19.56	88.50 ±3.51	0	3.10 ±0.003	0.94	0.01	0.06
10	*	*	2.90	3781.14 ±11.05	110.38 ±0.96	0	3.00 ±0.004	0.85	0	0.15

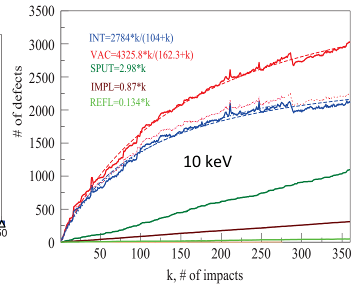
E≤1 keV,
Vacancies: A*k/(B+k)+C*k ,
Interstitials use the same A and B as in Vacancies, but notice C(negative) : A*k/(B+k)+C*k
Sputtering: D*k; Implantation: E*k; Impl2 (inty2): F*k; Refl: G*k

E>1 keV,
Interstitials: A*k/(B+k)+C*k ,
Vacancies use the same A and B as in Interstitials, but notice C(positive): A*k/(B+k)+C*k
Sputtering: D*k; Implantation: E*k; Impl2 (inty2): F*k; Refl: G*k

How to calculate fluence:
E≤1 keV,
Fluence=k*1.733126x10^{12}
E=2kev, E=4 keV:
Fluence=k*6.23925x10^{11}
E=6 keV, E=8 keV, E=10 keV:
Fluence=k*3.1832923x10^{11}

Significant fraction of "defects" located in surface layer, and
•contribute to surface roughening, rather than creating He trap sites.
:





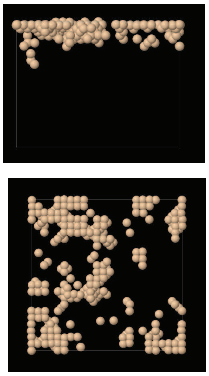
E (keV)	Spurt. yield	Implant. Yield	Reflect. probability
1	0.73	0.85	0.14
10	2.98	0.87	0.13

Krstic, 2013

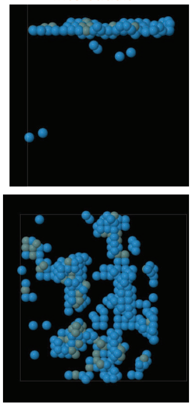
Defect clustering (1 kev, !000K)

After 888 impacts of W

Vacancies

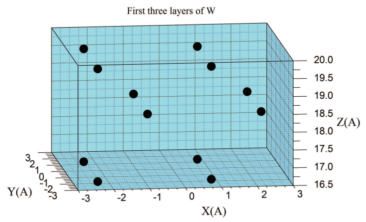


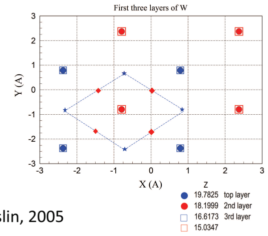
Interstitials



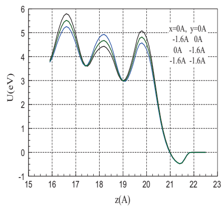
Krstic, 2013

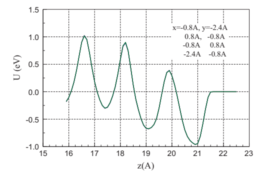
Perfect monocrystal of W



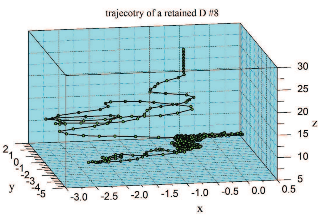


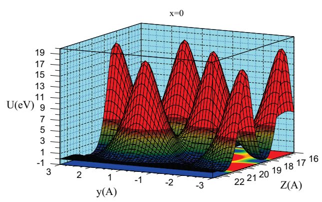
BOP of Juslin, 2005

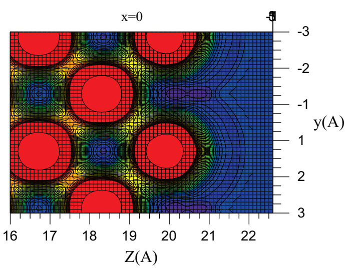


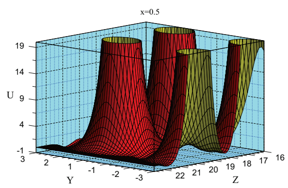


Krstic, 2014

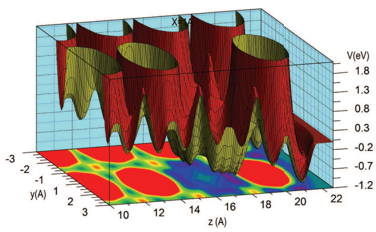


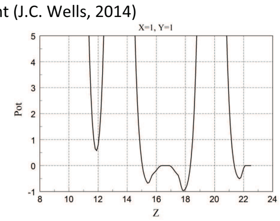


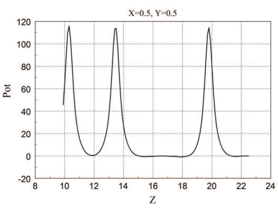


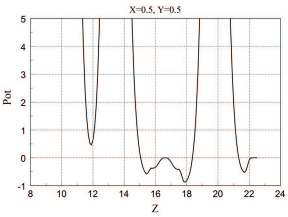


With a vacancy present (J.C. Wells, 2014)

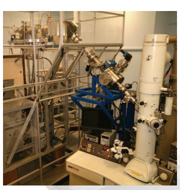


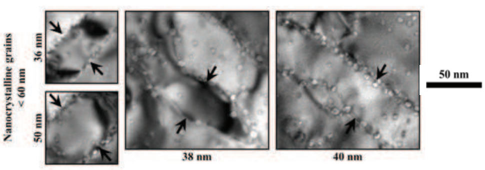


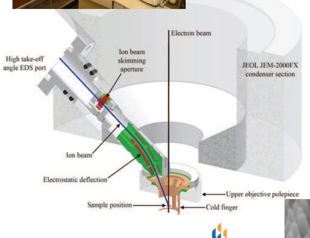




Fusion nanomaterials activities in Prof. J.P. Allain's research





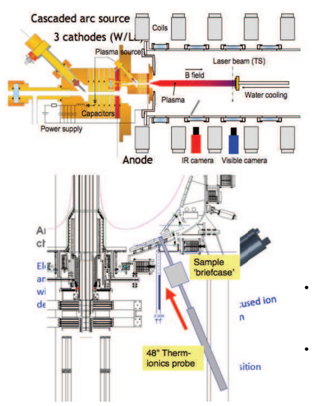


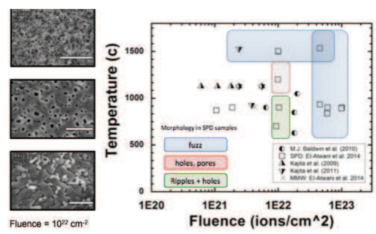
- Nanocrystalline tungsten work with in-situ TEM studying radiation resistant nanomaterials with Prof. Stephen Donnelly at the University of Huddersfield, UK.
- Prof. Allain to build IGNIS facility to study ion-induced nanopatterning on III-V systems at MNTL in collaboration with HZDR in Dresden, Germany

UIUC

University of HUDDERSFIELD

High-heat flux exposures of advanced extreme-refined tungsten in collaboration with DIFFER





- *In-situ* diagnostics of plasma-exposed surfaces using the new MAPP system in NSTX-U scheduled for first measurements in FY 2015 campaign
- High-heat flux exposures of lithium-coated tungsten and extreme-refined tungsten showing self-healing properties after high-temperature large fluence plasma exposure

J.P. Allain, UIUC

Lithium wall conditioning improves confinement! Why?

- We know from in-situ experiments labs, and more than 7 different tokamak machines (TFTR , CDX-U, FTU, DIII-D, TJ-II, EAST , and NSTX) that work with graphite with thin lithium coatings have a "significant" effect on plasma behavior and more specifically on hydrogen recycling.

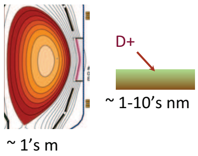
Controlled experiments demonstrated reduced recycling, improved energy confinement time t_E, and a reduction of edge instabilities known as edge localized modes (ELMs)

Notice the ratio of the dimensions of the plasma and Li layer!!!

How **fundamental** can we allow the theoretical physics of PMI to qualify it for an experimental validation?

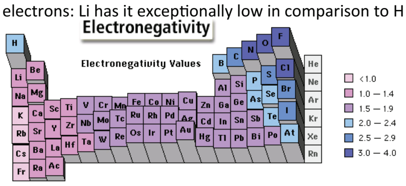
- Initially the experimentalists conjecture was that there was some "functionality" that governed the behavior of the Li-C-O-H system observed indirectly by analyzing the O(1s) and
- C(1s) peaks.

For "some reason" the Li(1s) peaks didn't show much information.

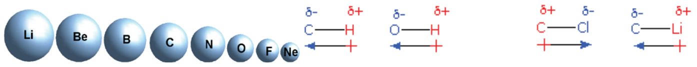


Lithium dynamics: Difficult to study theoretically by usual classical MD because Li polarizing features when interacting with other elements

Electronegativity is chemical property of an element defining its tendency to attract electrons: Li has it exceptionally low in comparison to H , C, O, Mo, W.

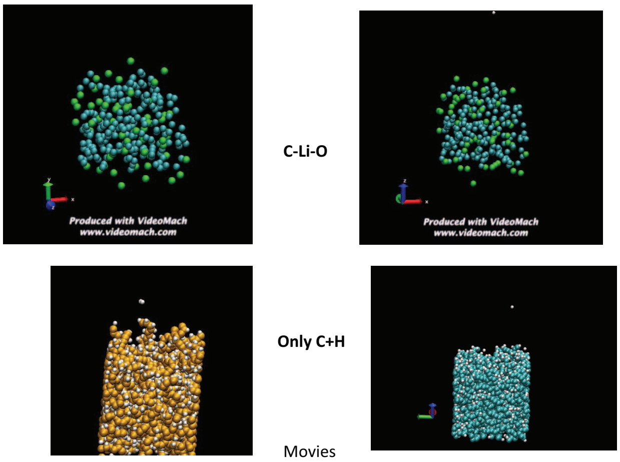


Consequence: Bonding between Li and other atoms covalent and polar;
Long-range nonbonding:
Coulomb :1/R
Lennard-Jones :$1/R^6$, $1/R^{12}$



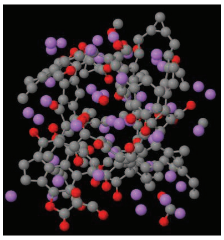
Quantum-Classical MD based on Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) method (developed by Bremen Center for Computational Mat. Science, Germany) a possible answer for qualitative phenomenology is our choice

Slabs studied: Periodicity in x-y



Movies

Simulation of deuterium impact to lithiated and oxidized carbon surface (quantum-classical approach, DFTB) Krstic 2012



- Cell of **a few hunreds atoms** of lithiated and oxidated amorphous carbon
- (~20% of Li, **and/or** ~20% of O), at **300K**

How?

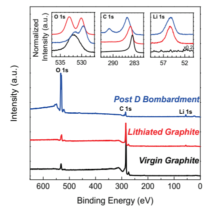
- By random seed of Li and O in **amorphous carbon** and **energy minimization**, followed by thermalization
- bombarded by **5 eV D** atoms, up to 500fs for the full evolution
- **Perpendicularly** to the shell interface
- 5004 **random trajectories** (embarrassingly parallel runs at Jaguar, Kraken); Time step **1 fs;** 30,000-50,000 CPU hours per run, number of runs > 10.

What do experiments teach us?

Experiments from Purdue (Allain, Taylor) and NSTX (PPPL) indicate higher retention and lower erosion rate with D whenever Li present in C, however XPS diagnostics show dominating D-O-C chemistry. Why – is the question now?

From experiments: There was correlation between hydrogen irradiation and the behavior change of the O(1s) and C(1s) peaks ONLY IN THE PRESENCE OF LITHIUM.

The Li(1s) peak was always invariant????

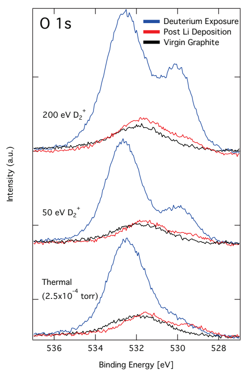


But theory says:

D has a slight preference for interacting with Li rather than with C.

Krstic et al., FED (2012)

How can we compare experiments and theory at all, when at such different energy scales?



Is it the impact energy problem?
QM model used 5 eV and experiment (cannot afford higher energy…)

Comes very interesting and theoretically anticipated result:

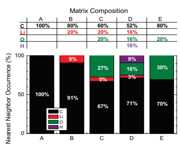
C. Taylor shows that the chemistry is incident particle energy independent… as expected.

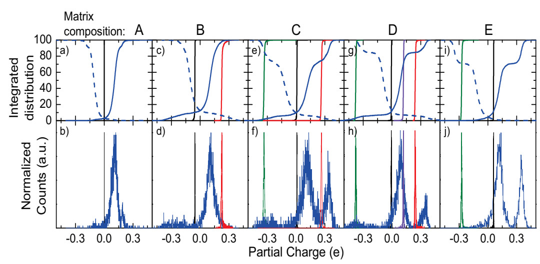
But, again a result came by observing the O(1s); in presence of Li
Not even the C(1s) showed much.

No problem with impact energy!!! Chemistry Evolves at thermal energy anyway!!!

How do Li and O compete?

OUR MODEL

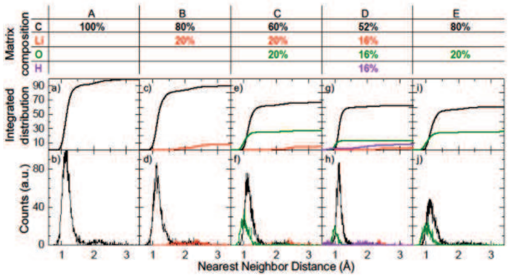




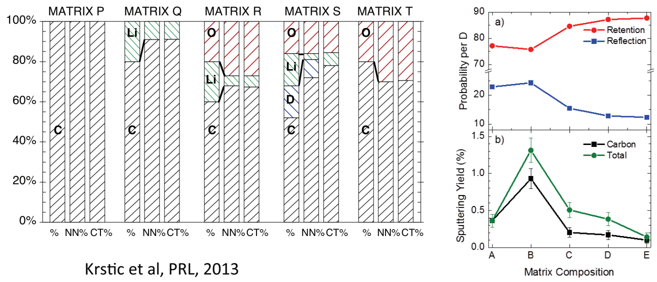
Indicate that D has a preference for interacting with O and C-O structures rather than with Li or Li-C structures **when there is enough O**

What do the first neighbors to D say?

Again: O preference!



What did theory teach us?



Krstic et al, PRL, 2013

If there is a SIGNIFICANT amount of oxygen on surface with lithium present in the graphite matrix, OXYGEN becomes the main player in retention-erosion chemistry; NOT LITHIUM!!!

What do experiments teach us? II

Here comes the experiment again (Chase):

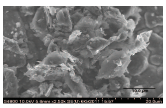
1) At most 5% oxygen content on the surface of NON-LITHIATED graphite... AS EXPECTED.

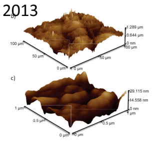
2) With lithium one gets 10% of Oxygen

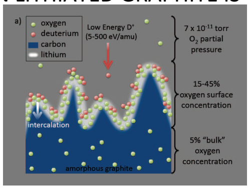
3) IMPORTANT: with LOW-ENERGY IRRADIATION one gets 20% oxygen and more on the surface.

..... B/C LITHIUM BRINGS IT THERE WHEN LITHIATED GRAPHITE IS IRRADIATED.

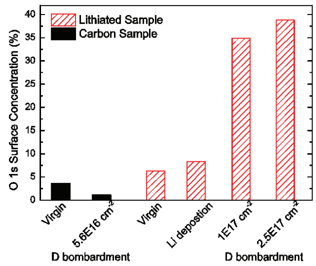
Taylor, Allain, 2013

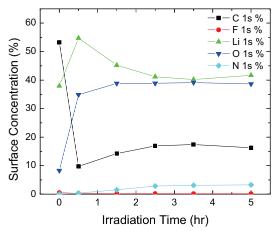






Supporting those finding:
Measurements of surface concentrations (C. Taylor, JP Allain)





Oxygen, carbon, and lithium concentrations at high deuterium fluences. The sample in this figure had a 2 μm nominal lithium dose deposited, after which XPS analysis showed an O(1s) oxygen concentration of 8.3%. Following deuterium irradiation of 30 minutes (9×10^{16} cm^{-2}) the oxygen concentration increased to 34.9%. Irradiation continued up to 5 hours (7.2 $\times10^{17}$ cm^{-2}). The oxygen surface concentration stabilized at ~ 38.8%. Interestingly, the apex of Li(1s) concentration occurs when the oxygen concentration has the largest increase.

What have we learned from both T&E?

It is not Lithium that suppresses erosion of C, and increases retention of H

OXYGEN plays the key role in the binding of hydrogen.

Lithium is the oxygen getter: Lithiation of C brings A LOT OF Oxygen inside C and this the main role of Li.

If there is a SIGNIFICANT amount of oxygen on surface with lithium present in the graphite matrix, OXYGEN becomes the main player; NOT LITHIUM!!! Oxygen and Oxygen-Carbon bond D strongly: suppressing erosion & increasing D retention.
... consistent with the XPS data!!

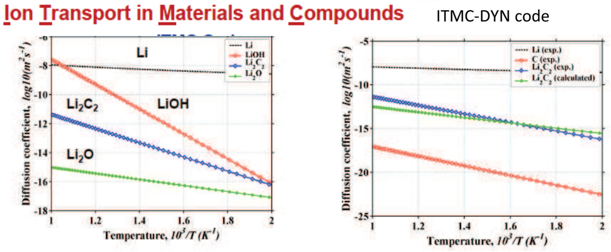
Krstic et al, PRL (2013)

Modeling of D interaction with Li and compounds

A. Hassanein

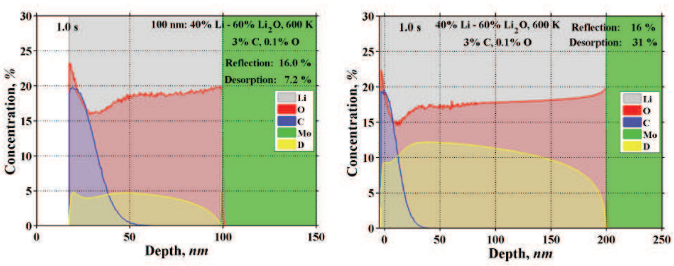
❑ **Three important processes for hydrogen interaction with liquid lithium surfaces – reflection, diffusion, and surface recombination.**

Ion Transport in Materials and Compounds ITMC-DYN code



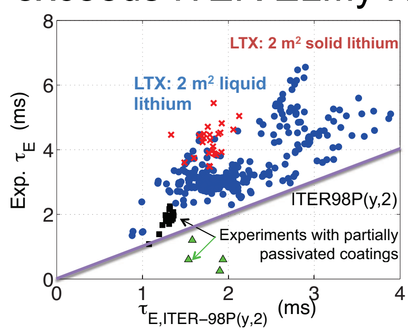
❑ **Using experimental results for hydrogen isotopes diffusion in Li and compounds, we estimated/calculated the diffusion coefficient in multi-component materials depending on target composition as the interpolation of logarithmic values of diffusivity in each compound.**

Deuterium Diffusion and Desorption in Contaminated Li Surface



❑ **Variation in initial Li compound thickness from 100 nm to 200 nm results in four times difference in deuterium desorption**

Confinement with lithium walls on LTX exceeds ITER ELMy H-mode scaling

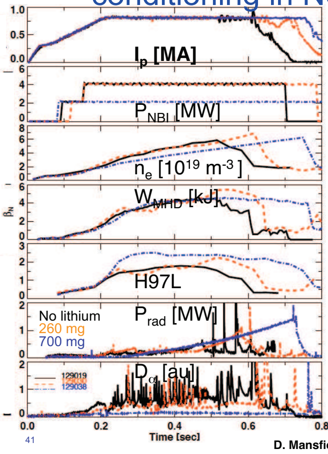


- Energy confinement exceeds ITER98P(y,2) by 3-4 x
- Less than 1% core lithium concentrations measured, even with full liquid lithium walls

R. Majeski, PPPL

- First operation of any tokamak with large area liquid lithium walls
- 2 m² of liquid lithium coated wall; 40% of plasma-facing surface
- Very recent experiments employ a full 4 m² liquid lithium wall

ELM-free H-mode induced by Li wall conditioning in NSTX (PPPL) R. Maingi



- Pre-Li, With-Li (260 mg), with-Li (700 mg)
- Lower heating power to avoid stability limit
- Lower n_e
- Similar stored energy
- Higher normalized energy confinement time
- Higher radiated power fraction
- Reduced divertor recycling, discharge ELM-free at higher dose

D. Mansfield, JNM 2009; R. Maingi, PRL 2009

Surface science elucidates plasma-wall interactions

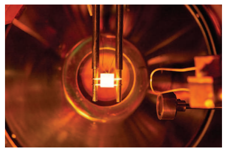
PRINCETON School of Engineering and Applied Science — PPPL PRINCETON PLASMA PHYSICS LABORATORY

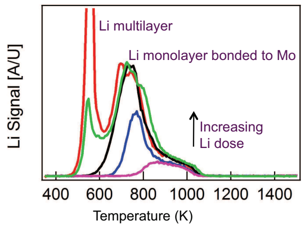
C.H. Skinner, A. M. Capece, J. P. Roszell, B. E. Koel,

- Plasma-wall interaction has profound affect on plasma performance, but the wall composition and morphology is hard to diagnose in tokamaks
- Surfaces under controlled conditions with well-defined particle flux and energies can be studied in the laboratory at the atomic scale
  - single crystal surfaces
  - monolayer control of film thickness
- Surface analysis systems can be attached to tokamaks for between-shot analysis.

MAPP probe end with four sample holders that can be heated independently JP Allain UIUC

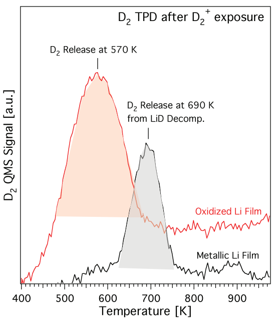
Temperature programmed desorption reveals Li-Mo chemical bonding.



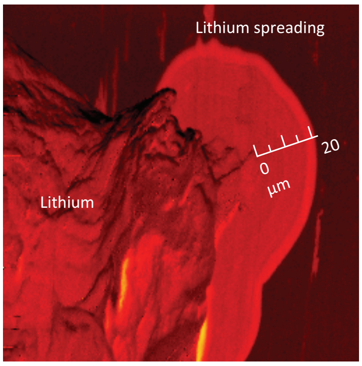


Surface science reveals details of D retention and Li wetting

Deuterium retention in lithium



Temperature programmed desorption shows oxygen inhibits formation of LiD and reduces thermal stability of D in Li films.

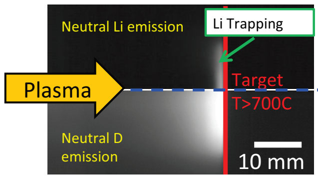


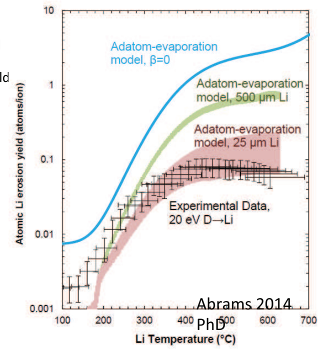
False color Auger image of lithium spreading over stainless steel at room temperature – relevant to wetting of liquid metal PFCs

Mixed-material and near-surface plasma effects indicate higher maximum surface temperatures may be feasible

- Mixed material effects in surface reduce gross erosion
  - Conversion to LiD depresses equilibrium Li vapor pressure
  - LiD concentration near surface leads to preferential D sputtering
  - Adatom damage and erosion model reproduces yield saturation
- Near-surface trapping results in large redeposition fraction and extended lifetime of thin (1μm) Li layer

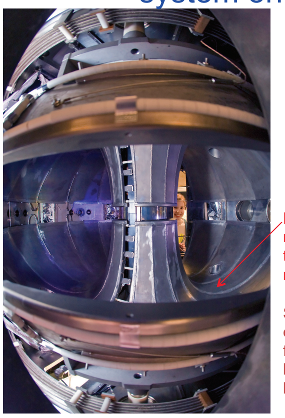
Li-I emission, t=2.5s



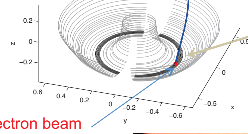


M. Jaworski 2014 PSI

New electron beam-based lithium deposition system on LTX (D. Majeski, PPPL)

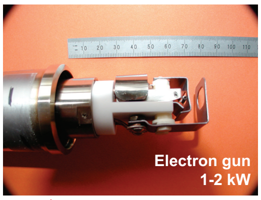


Beam system is mounted on upper vacuum vessel



Electron beam magnetically guided to lower shell lithium reservoir

Second e-beam evaporator produces full ($4\pi^2$) coating of liner with liquid lithium



Inner heated high-Z shell (explosively bonded SS on copper)

⇨ 2014: Fast (5 minutes for ~1000 Å) Li coating via electron beam evaporation

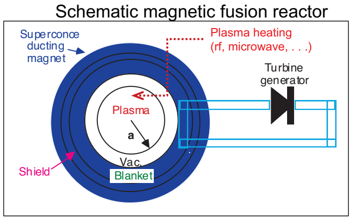
QUESTIONS:

Why PLASMA-MATERIAL INTERFACE is such an important problem?

All energy from D-T fusion reactions passes through first wall

- Flux of (particles + heat + 14 MeV neutrons) ~10 MW/m^2

Schematic magnetic fusion reactor



Why is PMI important?

- 17 Mev per d+t fusion in plasma core (> 50 mil. K) ; 80% transferred by n to Li blanket which fuel t; 20% carried by α, 1/4 supports the plasma, rest needs to be exhausted by e, p, α via atomic inelastic processes

Unlike nuclear fission where energy is volume-distributed

A FUSION REACTOR IMPLIES MANY INTERFACES BETWEEN THE PLASMA AND MATERIALS
Particles and surfaces

Key role of PMI in fusion research well recognized in US and internationally

The crucial role of the Plasma Material Interface (PMI) in fusion research is increasingly recognized

- 2007: DOE Greenwald Panel gap analysis for fusion
  *4 of 5 key knowledge gaps which must be bridged to achieve fusion power involve "taming the plasma-materials interface."
  *Importance of validating models that enable extrapolation from laboratory experiments to large devices.
- 2009: DOE Fusion Strategic Workshops recommendations
- In a 2013 report of the Fusion Energy Sciences Advisory Committee (FESAC), convened by DOE Office of Science Director, the research thrust "Decoding and Advancing the Science and Technology of Plasma-Surface Interactions" was identified as a top-5 priority in the US fusion strategy, including "*comprehensive theory-experiment comparisons in well-controlled and well-characterized conditions*, and *PSI evaluation of tungsten in appropriate **plasma, thermal, and radiation damage environments.***" [Extreme Reactor Conditions]
- DOE Office of Fusion Sciences (OFES) director Synakowski listed the understanding of materials in extreme fusion reactor environments as one of the two high-level goals in fusion research in the coming decade.
- A new OFES fusion materials science program is being developed with an ultimate goal of design and construction of the Fusion Nuclear Science Facility (FNSF).

Why science? Isn't it engineering?

or

How to build an effective science for PMI?

Guiding principle:

If Edison had a needle to find in a haystack, he would proceed at once with the diligence of the bee to examine straw after straw until he found the object of his search… I was a sorry witness of such doings, knowing that a little theory and calculation would have saved him 90% of his labor.

–Nikola Tesla, New York Times, October 19, 1931

The traditional trial-and-error approach to PMI for future fusion devices by successively refitting the walls of toroidal plasma devices with different materials and component designs is becoming prohibitively slow and costly !!

Need bottom-up approach arising from the fundamental atomistic and nano science

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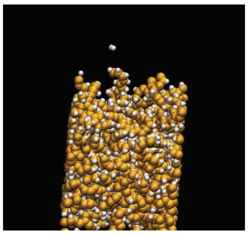
Why bottom-up science?

What does flux of 10^{25} particles/m^{2}s mean (ITER) for a typical atomistic (MD) simulation?



At a box of surface of 3 nm lateral dim?
a few thousands atoms (carbon)

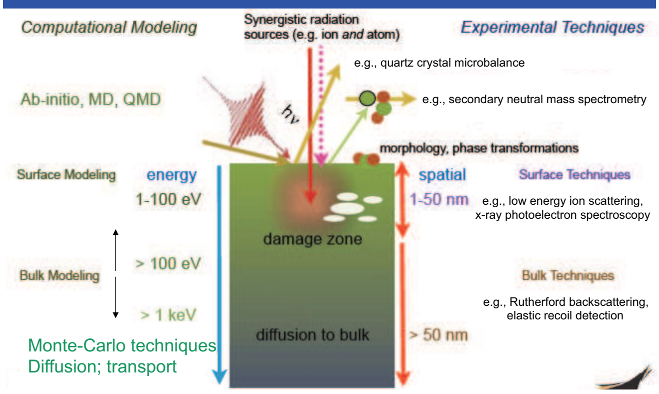
The flux is 0.01 particle/nm^{2}ns
1) 1 particle at the interface surface of the cell each 10 ns.

But for deuterium with impact energy less then 100 eV: Penetration is less than 2 nm, typical sputtering process takes up to 50 ps

Is each impact independent, uncorrelated?

Each particle will functionalize the material, change the surface for the subsequent impact!
Processes essentially discrete → Atomistic approach (bottom!!!)

Probing the PMI requires integration of many experimental and theoretical techniques spanning orders of magnitude in time, length, and energy scales



Courtesy of J.P. Allain

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Computational TOOLS for atomistic approaches

http://lammps.sandia.gov

LAMMPS is classical molecular dynamics code For ensemble of particles in a liquid, solid, or gaseous phase

Highly efficient, GPU functionality recently too
Highly parallelized, up to millions of atoms

…And KMC… (in various versions)

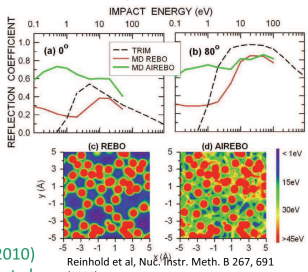
Classical MD is only as good as the interatomic potential model used

Most advanced: hydro-carbon potential developed for chemistry
- Brenner, 1990 , 2002 : REBO, short range, 0.2nm
- more sophisticated AIREBO (Stuart, 2000, 2004, 1.1 nm)
- > 400 semi-empirical parameters, "bond order", chemistry

Adaptive Intermolecular Reactive Bond Order (AIREBO) potential : torsion, dispersion, Van der Waals,
Even for hydrocarbons problems visible

EX: MD calc. of reflection coeff.
- **Significant sensitivity to changes in potential model for some processes**
- Experimental validation essential to establish credible MD simulation.
- Interatomic potentials for W, Be, C exist (Nordlund, Juslin (W,H,C<He)
- Experimental validation? So far good!

Notice the problem with TRIM!



Reinhold et al, Nucl. Instr. Meth. B 267, 691 (2009).

Improvements to CH potentials done (Kent et al, 2010)
New Li-C-H-O potentials being developed (Dadras et al, 2010)

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If PMI is so important why it took decades to have its importance recognized?

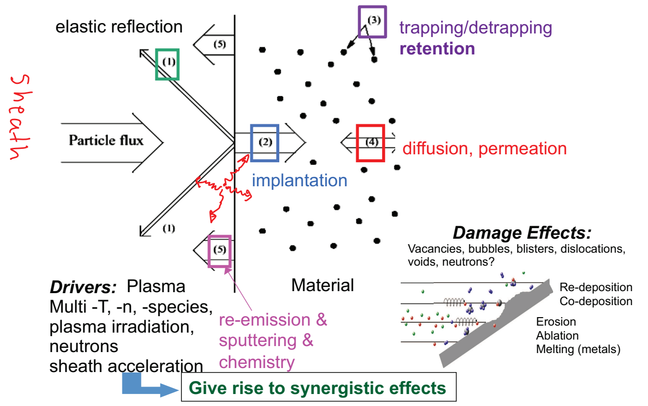
Off-hand: Because it is too difficult?
Then, why is PMI so difficult problem?

Answer: Interfacial physics, "when the two worlds meet" : traditionally the most challenging areas of science

Dynamical surface communicates between two worlds: Plasma and Material

PMI has many fundamental processes & synergies

When an ion or neutral arrives at a surface it undergoes a series of elastic and inelastic collisions with the atoms of the solid.



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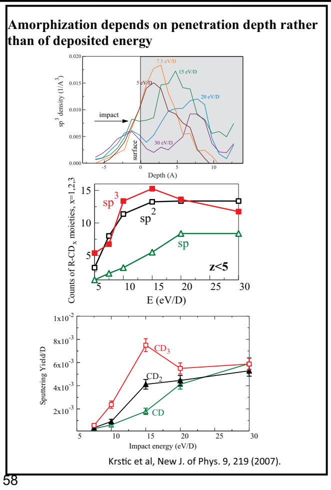
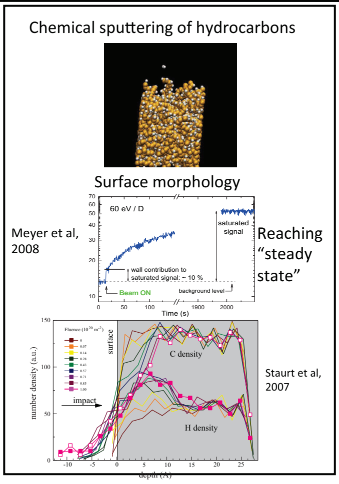
Materials exposed to plasma are modified, resulting in a "dynamical" surface





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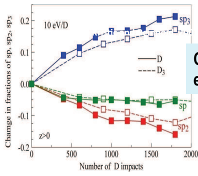
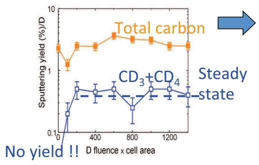
"dynamical" surface

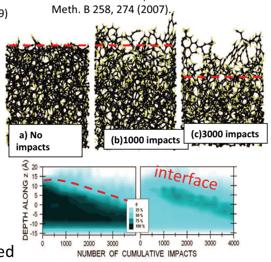


Chemical structure (hybridization sp/sp^2/sp^3) of surface evolves under hydrogen bombardment

Krstic et al, Nucl. Instr. Meth. B 267, 704 (2009)

C. O. Reinhold et al, Nuc. Instr. and Meth. B 258, 274 (2007).



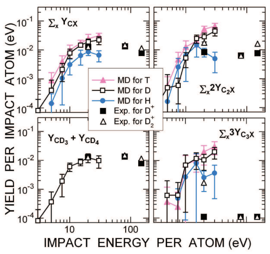


Steady state of sputtering formed

How to validate theory with experiments (and vv) at the PMI interface called "surface"?

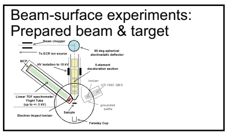
What have we learned from the "next door" beam-surface experiments?

Beam-surface exp't: precision control of projectiles & targets . . .
. . . enabled development & validation of MD approach



Remarkable agreement of theory & exp't when simulation mimics exp't. No fitting parameters!

Key: simulation prepares surface by bombardment!
- Fluence (not flux) like that in experiment
- Type, internal state, energy, angle as in exp't



Meyer et al, Phys. Scripta (2007);
Krstic et al, NJP (2007)

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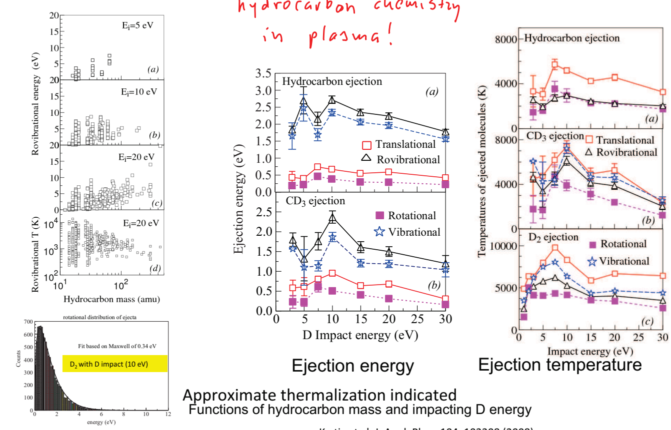
But once validated
Theory can Provide a New Physics not accessible by Exp.

hydrocarbon chemistry in plasma!



Ejection energy

Ejection temperature

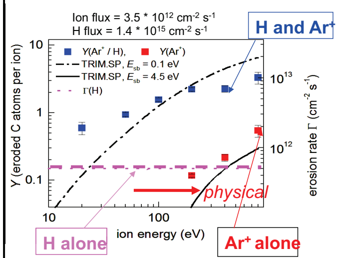
Approximate thermalization indicated
Functions of hydrocarbon mass and impacting D energy

Krstic et al, J. Appl. Phys. 104, 103308 (2008).

Do we need "special" plasma irradiation?
Why?
How to treat irradiation of plasma computationally?

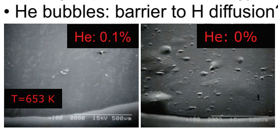
Because of synergy in the evolution of surface irradiated by plasma

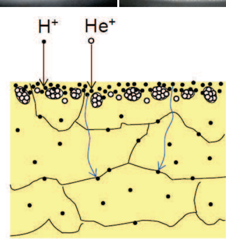
Experiments with Ar+ and H:
- Sputtering = (chemical) + (physical)
- Surface preparation by H impact for chemical sputtering
- Impurity atoms in plasma are efficient precursors for erosion
- PM processes very dependent on inventory of H in the material



Hopf & von Keudell, 2003

He suppresses H retention in W
- He penetrates deeper than H
- Strong dependence on energy
- He bubbles: barrier to H diffusion?

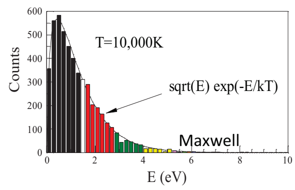


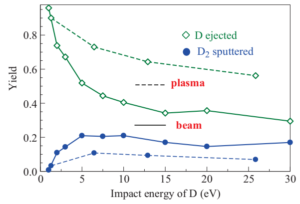


R. Doerner et all and others

Simulations of the plasma irradiation (D atoms)

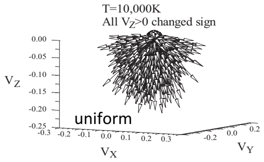
HOW?





Krstic et al, 2009

Impact distributions



With plasma irradiation:
Reflection significantly higher than with beam,
But sputtering is suppressed !!!

Computationally intensive but necessary!

What is outreach of the PMI science at the plasma facilities?

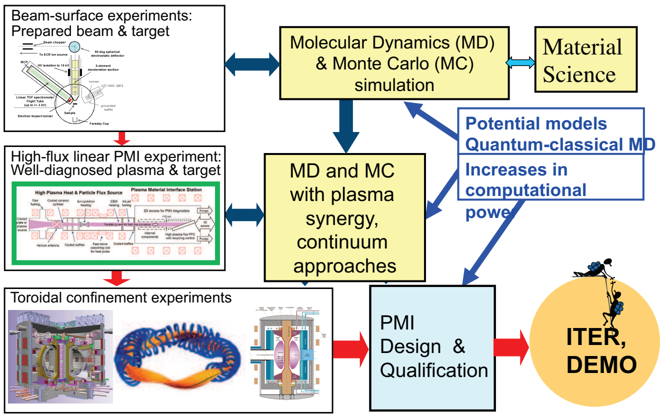
or

Is there a need for dedicated PMI plasma facility?
Answer is obviously “”YES”!
What do we want to do with it?

Difficult to study PMI in thoroidal facilities !

Importance of the dedicated PMI facilities Pisces-B, Magnum, …) = Bridge!!!

Integration of theory & experiment⇒ basis for PMI research



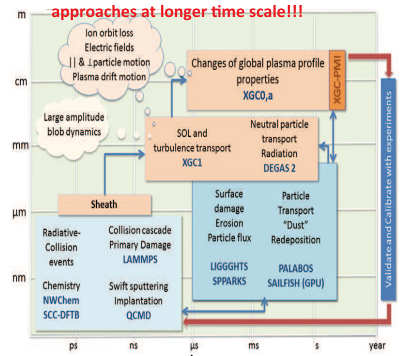
Predictive science!!!

What is a single, most important problem in PMI for fusion?

Strategic objectives for theory: Integrated plasma & material modeling system: Most important!!!

Plasma codes resolve events at the scale of μs

At shorter than μs time: Study phenomenology, provide parameters for MC approaches at longer time scale!!!



Atomistic PMI codes (Computational chemistry NWChem, Approximate DFT: SCC-DFTB, Quantum-Classical Molecular Dynamics, Classical Molecular Dynamics, LAMMPS)

Mesoscopic PMI codes (DEM: LIGGGHTS and KMC:SPPARKS, referenced in the text, and Lattice-Boltzmann codes [PALABOS] and [SAILFISH]),

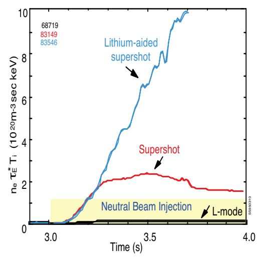
Plasma codes (XGC family and DEGAS 2)

Study PMI separately, with plasma drivers

Integration of PMI and plasma at the "same footing", with nano PMI drivers

Effect of Tokamak Wall Conditions on Core Plasma Performance Not Understood

- Tokamak operation contingent on empirical wall conditioning techniques, such as boronization.
- Most dramatic effect: application of Li on TFTR.
- Subsequent examples of beneficial effects of Li include CDX-U & NSTX.
- Conditioning techniques generally reduce D & impurity influx,
- Why these are beneficial for core plasma is not understood.
  – Some effect on core turbulence?
- Diagnostic & run time limitations make purely experimental investigation prohibitive.
- ⇒ use1st principles (or nearly so) coupled PMI + plasma turbulence code to provide deeper insight,
- EPSI SciDAC project dedicated to latter objective,
- We propose to develop the former.



D. Stotler, PPPL, 2014

“State of the Art” Plasma Simulation Codes Use Rudimentary PMI Models

- SOLPS = B2 (2-D fluid plasma transport) + EIRENE (3-D kinetic neutral transport) used to simulate JET, design ITER, etc.
  – Reflection, physical sputtering data from TRIM (BCA) calculations,
  – User specified absorption coefficients,
  – Empirical or calibrated chemical sputtering yields.
- UEDGE (2-D fluid plasma transport) & XGC (kinetic plasma turbulence & transport) use specified recycling coefficients,
  – Can be coupled to DEGAS 2 kinetic neutral transport to use TRIM reflection data.
- PMI do not evolve in response to plasma ⇒ no consistent solution to plasma-material system.
- Replacing with dynamic, first principles, multi-scale model:
  – Consistent treatment of D retention & recycling,
  – Surface morphology evolution through erosion & redeposition,
  – Kinetic characterization of impurity sources,
  – Etc.

Quality assurance in PMI?

What is Uncertainty Quantification?

•Propagate uncertainties in input variables, parameters and models to quantify effects on output metrics

–Essential for incorporating outputs of physical models into engineering design/decision processes

–Guides research activities and investments

–Rigorous derivation of coarse-graining schemes

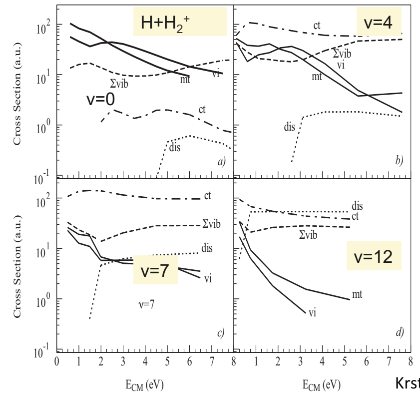
Inputs x (observables, parameters, initial conditions, model, ...) → Computational model f(.) → Outputs f(x) (metrics, failure probabilities, decisions, design points,...)

Total uncertainty: input + modeling + numerical + statistical

- Aleatory uncertainty: inherent or irreducible (e.g., radioactive decay)
- Epistemic uncertainty: reducible in principle (e.g., incomplete models)

We need all processes at the same footing!!
FOR CONSISTENCY AND UNITARITY

"Interplay" of transport and inelastic processes



Krstic, 2003

7a/31/14

Example: How the same footing works!

Community Agitation

•UQ is widely applied in engineering

–e.g., nuclear reactor design, construction, ...

•and a few science domains, e.g., climate

•but is largely absent in the physical sciences

–a few groups are pursuing this, but it needs to become pervasive

•Workshop on UQ in physics/chemistry

–Organizing committee so far: Gordon Drake, Petr Plechac, Daren Stottler, Bas, PK, RJH

–Bring together mathematicians + scientists

–Proposed for late spring(?) 2015 in/near NYC

R. Harrison, IACS, Stony Brook

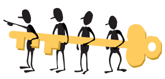
CONCLUSIONS

What have we learned from studies of surfaces, i.e. interfaces of plasma and materials?

- PMI extremely difficult interfacial problem (Material mixing create SURFACE entity; its scale depends on impact energy: For sub-100eV => nm-ns scales
- PMI science can be built from bottom-up recognizing its multiscale character and building from shortest time/spatial scales (fs/Angstrom) up
- Theory&modeling of PMI must be validated by experiment (and v.v.), the qualitative understanding on phenomenology rewarding
- Irradiation create dynamical surface, changing interface, cumulative bombardment is the key for agreement with experiment
- Surface responds to synergy in plasma irradiation (angles, energies, particles), NOT following linear superposition principle; Plasma irradiation modeling and experiments with beam experiments.
- Chemistry&dynamics of lithiated and oxygenated surfaces must be treated by QM -> QCMD
- Self-healing feature of tungsten defects upon cumulative bombardment of ions and "neutrons"; clustering; nanograining.

Looking forward

- The plasma-material interface has a big effect on the plasma performance, and we don't understand why!
  The answers can be found in the plasma-PMI integration science.
- The main weight in the science of integration of fusion plasma and its interfacial surface boundaries is carried by PMI because 1) the basic PMI phenomenology evolves much faster than the plasma time scale, and 2) it evolves through wider range of the scales, which partially overlap with the scale of plasmas. The PMI has to be understood and parameterized at nanoscale before integrating it with plasma at the "same footing" at micro-scale.
- Bringing together the various scales of PMI and plasma is the fundamental multisdisciplinary question, covering plasma science, surface science, atomic physics, computer science and applied mathematics.
- The team of physicists, computer scientists and mathematicians is needed to perform the multiscale, integration task. Need to do from low Z to high Z, from liquid metals to polycrystals, chemical and physical processes. Computer resources, computer codes, knowledge "how-to" are available. Funding the PMI-plasma integration science would avoid trail-and-error loses and save millions of dollars.
- UQ and Quality validation of the simulations is the key for the "right track". Mimicking the experiments by simulation is the key for the successful validation. High quality experiments, well suited for the purpose do exist.



Our thanks to John Hogan (FED, ORNL)

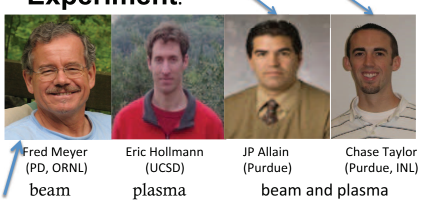
H. Witek, Taiwan

Many thanks to PMI close collaborators:

Theory: CMD Mat. PWDFT **TBDFT modeling**

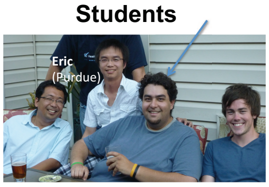
Carlos Reinhold PD, ORNL — Steve Stuart Clemson U. — Paul Kent ORNL — Alain Allouche CNRS, Fr — K. Morokuma, Kyoto U. — J. Jakowski, NICS — S. Irle, Nagoya U

Experiment:



Fred Meyer (PD, ORNL) beam — Eric Hollmann (UCSD) plasma — JP Allain (Purdue) — Chase Taylor (Purdue, INL) beam and plasma

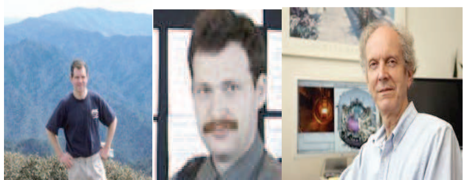
Students



Jae (ORISE) PhD — Jonny (UTK) PhD — Chris (MTSU)

Jeff Harris, Rick Goulding, FED, ORNL

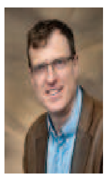
Tungsten, present **PPPL**



Daren Stotler — Igor Kaganovich — Charles Skinner

Many thanks

IACS **IAPCM** **CCS-ORNL**



Robert Harrison

Yong Wu

THANK YOU!