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)

![Image of fusion in stars]

the energy release rate in sun is only 276 μW/cm²

Impractical for terrestrial conditions

Fusion on earth (Controlled fusion!)
• d-fusion (more efficient)
T=150 mil K
• Alpha-particles and neutrons carry most of the energy

Challenges with tungsten in fusion
Neutron inflicted defects
• 14 MeV Neutrons? Energetic particles?
High Temperatures!
For realistic energy conversion (DEMO) need a hot surfaces > 600°C
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)

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 loss of nanometer sized grains that is independent of surface grain orientation. But there is still no coherent picture of why flux thresholds exist and what its defining factors are
• For He-ion impact energies below displacement damage threshold, growth of nanostructures due to the impingement of intrinsic or extrinsic defect sites with subsequent dynamics of near-surface cluster nucleation, bubble formation, coalescence growth, and ultimately burning, 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.

Previous Nano-fuzz Research
• First investigations of nano-fuzz production on hot tungsten surfaces by He-ion exposure were performed with linear plasma devices – MAGDOS, PILOT-PSI, and PIECS-B – with ion energies below 200 eV (But broad energy distribution):
  - Nano-fuzz formation observed for fluxes > 10¹⁰ m⁻² s⁻¹ and T > 1100 K
  - Nano-fuzz thickness grew as square-root of exposure time, interpreted as diffusive mechanism

• Investigation at NERF 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 10¹⁰ m⁻² s⁻¹ and T > 1100 K

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

![Image of plasma impact and conditions]

Bannister, Meyer, ORNL
As bubbles continue to grow at very high pressure, eventually rupture mobile, strongly bound helium clusters change) fusion devices (e.g. during disruptions, Mass loss would have significant Reduced tendril density after dual exposure. due to enhanced sputtering? He impact on tungsten away from normal normal incidence exp. (1) +1 2 02 +1 2 beam approach (currently)! only possible using ion study. Hennion and Web, UT/CRNL Due to enhanced sputtering? He \( \text{exp. (2)} \)

**Tungsten surface response to low-energy He exposure**

- 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 (I: MD 10\(^{18}\) vs exp 10\(^{19}\); \( \Phi \): 10\(^{20}\) vs 10\(^{21}\))

**MD simulation of self-atom damage 1 keV**

- 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

**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
- 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

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

<table>
<thead>
<tr>
<th>( \text{One way to study impact of 14 MeV neutrons and other light energetic particles} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sqrt{M_{\text{He}}} )</td>
</tr>
<tr>
<td>( \text{Exp:} ) Virgin W has very low density of intrinsic defect sites at which to trap He</td>
</tr>
<tr>
<td>He trapping during subsequent He ion exposures, perhaps even amorphize surface, and/or accelerate fuzz growth, but effect is small</td>
</tr>
</tbody>
</table>

**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

**Nano-fuzz Formation Still Not Understood**

A number of explanations proposed:
- Pinhole formation
  - Kraja et al., JNM 2011
  - Krachmalnikov, Phys. Script. 2013
  - Lase et al., JNM 2015
- “Visco-elastic” growth model
  - Viscous W flow gives square-root of fluence dependence
  - Qualitative only
- Need nano-fuzz measurements performed under well-characterised and well-defined conditions

**Experimental W self-ion fluence**

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

**MD data**

10 keV W

**Krstic**

**Krstic**

**Krstic**
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
Spattering: D^{*}k; Implantation: E^{*}k; Impl2 (inty2): F^{*}k; Refl: G^{*}k
E=1 keV, Interstitials: A^{*}k/(B+k)+C^{*}N,
Vacancies use the same A and B as in Interstitials, but notice C(positive): A^{*}k/(B+k)+C^{*}k
Spattering: D^{*}k; Implantation: E^{*}k; Impl2 (inty2): F^{*}k; Refl: G^{*}k

How to calculate fluence:
E=1 keV, Fluence=k\cdot1.73312k/10^{12}
E=2keV, E=4 keV:
Fluence=k\cdot6.23925k/10^{11}
E=6 keV, E=8 keV, E=10 keV:
Fluence=k\cdot3.18329k/10^{11}

Significant fraction of “defects” located in surface layer, and
* contribute to surface roughening, rather than creating trap sites.

Defect clustering (1 kev, 1000K)
After 888 impacts of W

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

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

In-situ plasma nanosynthesis

In-situ high-temperature large fluence plasma exposure

High-heat flux exposures of lithium-coated tungsten and

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

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 Sweden, Germany.

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

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

Electronegativity is a 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^2, 1/R^1

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

C-Li-O

Only C-H

Movies

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

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, Ti-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_c, and a reduction of edge instabilities known as edge localized modes (ELMs).
  
  Notice the ratio of the dimensions of the plasma and Li layer!!!

- 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.

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

- Cell of a few hundreds of lithiated and oxidized 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
  - Bonded 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., FEO (2012)

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

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!!!
What do the first neighbors to D say?
Again: O preference!

What do experiments teach us?
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.

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!!

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

- Energy confinement exceeds ITER88P(y,2) by 3-4 x
- Less than 1% core lithium concentrations measured, even with full liquid lithium walls
- 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

Supporting those findings:
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 (3×10²⁰ D/cm²) the oxygen concentration increased to 34.9%. Irradiation continued up to 5 hours (3.2×10²¹ D/cm²). The oxygen surface concentration stabilized at ~38.8%. Interestingly, the apex of Li(1s) concentration occurs when the oxygen concentration has the largest increase.

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

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

Deuterium retention in lithium

Lithium spreading

Lithium

Lithium

Lithium

Neutral Li emission

Li Trapping

Plasma

Target

Neutral D emission

Abrams 2014

M. Jaworski 2014 PSI

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

- Flux of (particles + heat + 14 MeV neutrons) ~10 MW/m²

Why is PMI important?

- 17 MeV per d-t fusion in plasma core (50 mJ/Å); 80% transferred by n to Li blanket which fuel is 20% covered by α. 1/4 supports the plasma, rest needs to be exhausted by α, β, etc. via atomic inertial processes

Schematic magnetic fusion reactor

Why is PMI important?

Unlike nuclear fission where energy is volume-distributed

A FUSION REACTOR IMPLIES MANY INTERFACES BETWEEN THE PLASMA AND MATERIALS

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 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 P1/P0 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).

QUESTIONS:

Why PLASMA-MATERIAL INTERFACE is such an important problem?

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
**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 refining 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

**What does flux of \(10^{15}\) particles/m²/s mean (ITER) for a typical atomistic (MD) simulation?**

- At a box of surface of 3 \(\text{nm}\) lateral dim?
  - a few thousands atoms (carbon)

- The flux is 0.01 particle/\(\text{mm}^2\)/ns.
- 1) 1 particle at the interface surface of the cell each 10 ns.

- But for deuterium with impact energy less than 100 eV: Penetration is less than 2 \(\text{nm}\), 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  🟢  Atomic approach (bottom!!!)

**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)

**Why bottom-up science?**

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 hydrocarbon 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!

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

Notice the problem with TRIM!

**Why science? Isn’t it engineering?**

or

**How to build an effective science for PMI?**
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.

**Drivers:** Plasma, Multi-T, n., species, plasma irradiation, neutrons, sheath acceleration

**Material:** Implantation, re-emission & sputtering & chemistry

**Damage Effects:** Vacancies, radiation defects, dislocations, voids, neutrons?

- Re-deposition
- Co-deposition
- Erosion
- Ablation
- Melting (melts)

**Chemical re-emission &**

Give rise to synergistic effects

**Sputtering =**

(chemical) + (physical)

PM processes very dependent on

Surface preparation by H impact for

He: 0%

Impurity atoms in plasma are efficient

beam-surface experiments?

What have we learned from the “next door”/g14/g32/g62/g32/g50/g1/g32/g52/g1/g28/g44/g68/g1/g17/g40/g62/g51/g71/g1/g1/g20/g30/g50/g41/g48/g52/g28/g1/g1/g80/g93/g91/g91/g98/g81/g69/g1

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Key: simulation prepares surface by bombardment!

parameters!

When simulation mimics exp’t. No fitting

Remarkable agreement of theory & exp’t

when simulation mimics exp’t. No fitting parameters!

Type, internal state, energy, angle as in exp’t

Meyer et al, Phys. Scripta [2007];

Krstic et al, NUP [2007]

Because of synergy in the evolution of surface irradiated by plasma

- 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

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

Approximate thermalization indicated

Functions of hydrocarbon mass and impacting D energy


Do we need “special” plasma irradiation?

Why?

How to treat irradiation of plasma computationally?

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

Amorphization depends on penetration depth rather than of deposited energy

Chemical sputtering of hydrocarbons

Reaching “steady state”

What have we learned from the “next door”/g14/g32/g62/g32/g50/g1/g32/g52/g1/g28/g44/g68/g1/g17/g40/g62/g51/g71/g1/g1/g20/g30/g50/g41/g48/g52/g28/g1/g1/g80/g93/g91/g91/g98/g81/g69/g1

61

Beam-surface experiments. Prepared beam & target

Meyer et al, Phys. Scripta [2007];

Krstic et al, NUP [2007]

**“dynamical” surface**

Chemical structure (hybridization sp/sp/sp<sup>3</sup>) of surface evolves under hydrogen bombardment

How to validate theory with experiments (and vv) at the PMI interface called “surface”??
High-flux linear PMI experiment:

Beam-surface experiments:

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

Integration of theory & experiment⇒ basis for PMI research

Material Science

Potential models
Quantum-classical MD

Increases in computational power

MD and MC with plasma
synergy, continuum approaches

Molecular Dynamics (MD) & Monte Carlo (MC) simulation

PMI Design & Qualification

 ITER, DEMO

Predictive science!!!

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!!!

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

Mesoscopic PMI codes
(DEM: UGGSHTS and KMC-SPPARX, 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

“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 (BCC) 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,

Quality assurance in PMI?

Effect of Tokamak Wall Conditions on Core Plasma Performance Not Understood

• Tokamak operation contingent on empirical wall conditioning techniques, such as ionization.
• Most dramatic effect: application of Li on TFR.
• Subsequent examples of beneficial effects of Li include COEX-L & NIXE.
• 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.
• ⇒ use “in” principles (or nearly so) coupled PMI + plasma turbulence code to provide deeper insight,
• EPS-SeDAC project dedicated to latter objective,
• We propose to develop the former.

D. Stotler, PPPL, 2014

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!!!
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 \( f(\cdot) \)

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)

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 Strottler, Bas, PK, RJH
  - Bring together mathematicians + scientists
  - Proposed for late spring(?) 2015 in/near NYC

R. Harrison, IACS, Stony Brook

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 energy: For sub-100eV \( \gg \) nm-ns scales
- PMI science can be built from bottom-up recognizing its multiscale character and building from shortest time/spatial scales (fs/Ångstrom) 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 \( \Rightarrow \) 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 multidisciplinary question, covering plasma science, surface science, atomic physics, computer science and applied mathematicians.
- 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 trial-and-error losses 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.
THANK YOU!