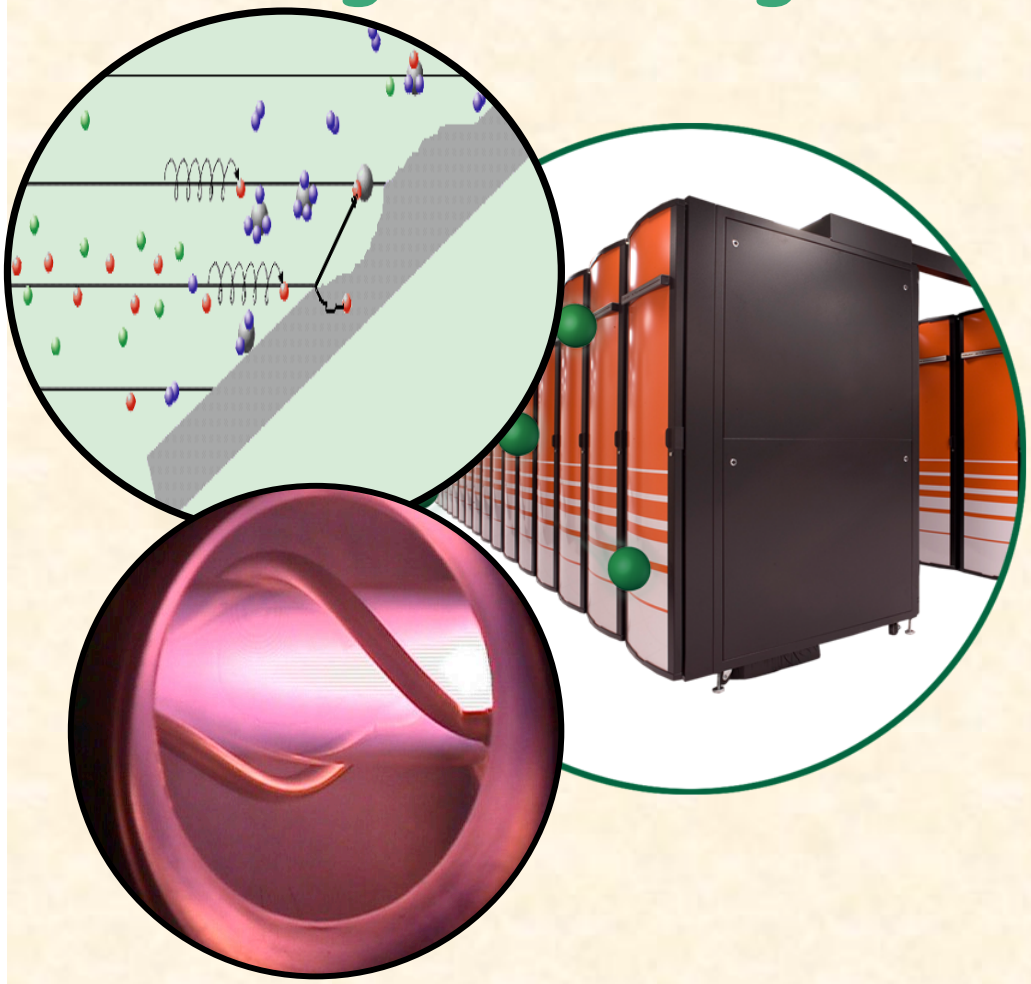
Plasma-Material Interface: Giga Challenge For Fusion Energy



Predrag Krstic

Physics Division, CFADC
Oak Ridge national Lab
Oak Ridge TN, USA

Supported by DOE OFES & OBES, SciDAC, INCITE

Close collaborators:

Theory:

Carlos Reinhold (PD)

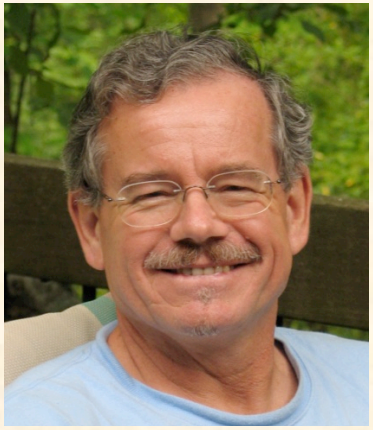
Steve Stuart (Clemson U.)

Paul Kent (CNMS)

jpg

Our thanks to John Hogan (FED, ORNL)

Experiment:



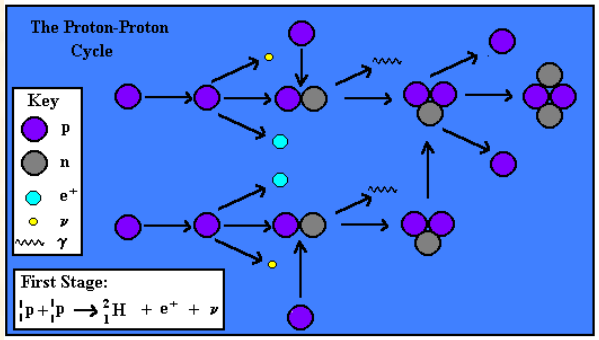
Fred Meyer (PD)
beam

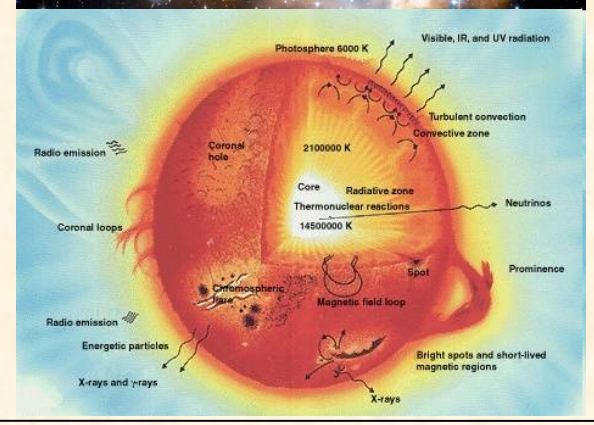
Eric Hollmann (UCSD)
plasma

Astro-fusion against terrestrial fusion?

Fusion in stars

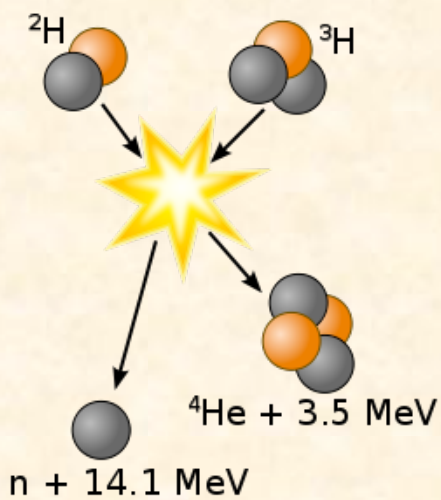
•Process in the core of our Sun and stars: H atoms fuse into He (T=15 mil)





the energy release rate in sun is only 276 μW/cm^3

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

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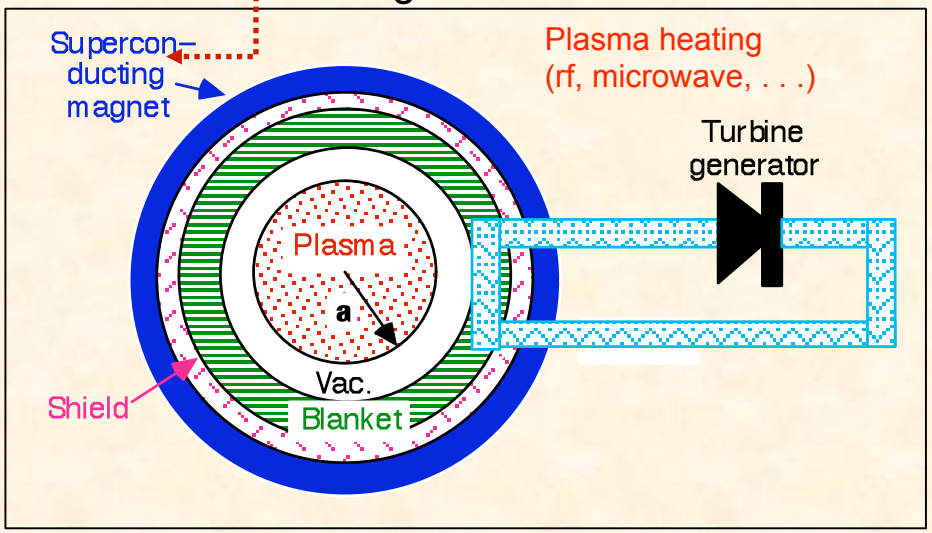
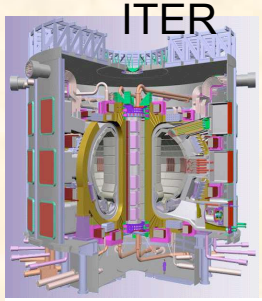
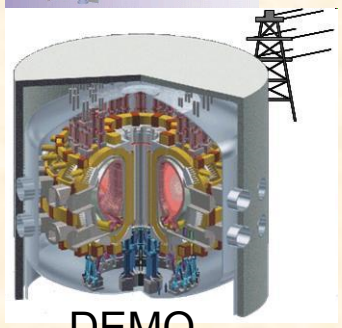
All energy from D-T fusion reactions passes through first wall

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

Schematic magnetic fusion reactor







Unlike nuclear fission where energy is volume-distributed

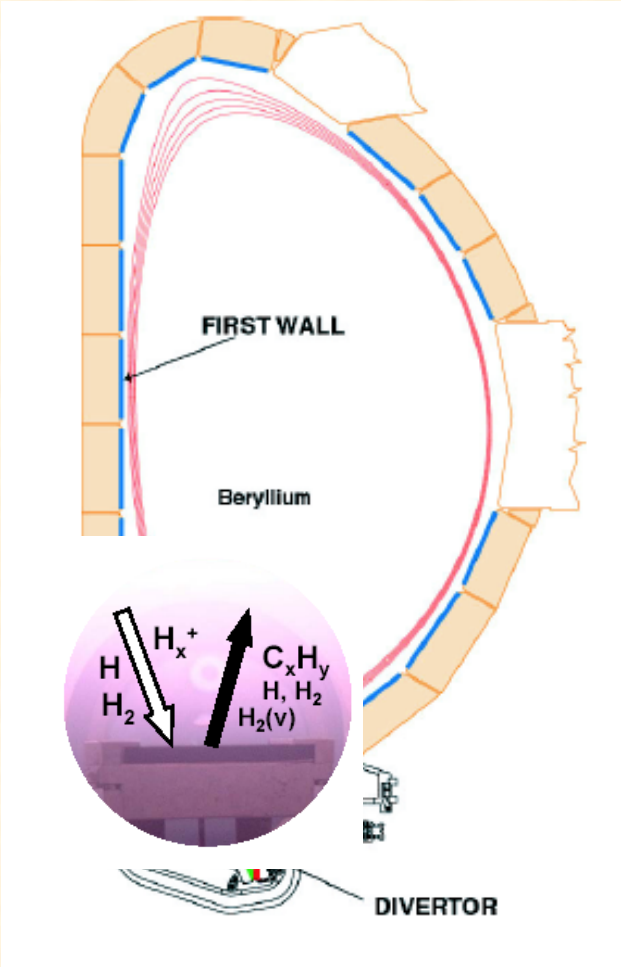
ITER: Biggest international sci project of present times

EU, Japan, Russia, China, Korea, US, India partnership, 30 year agreement

ITER ranked 1st for US Investment of facilities in next 20-years (2003)
Strongly supported by all US scientific and educational entities

Princeton/ ORNL partnership manage project office for US ITER activities

PMI strategy is evolving thru ITER towards DEMO reactor



Divertor: Magnetic filed lines end – biggest flux of particles & energy

ITER (> 2020) uses multi-matl walls

Pulses ~ hundreds of sec

~Be Main chamber wall(700m^2)

Low Z + oxygen getter

~W Baffle/Dome (100 m^2)

Low erosion, long lifetime

~ C Divertor Target (50 m^2) (Graphite)

Minimize high-Z impurities

(which lead to large radiative losses)

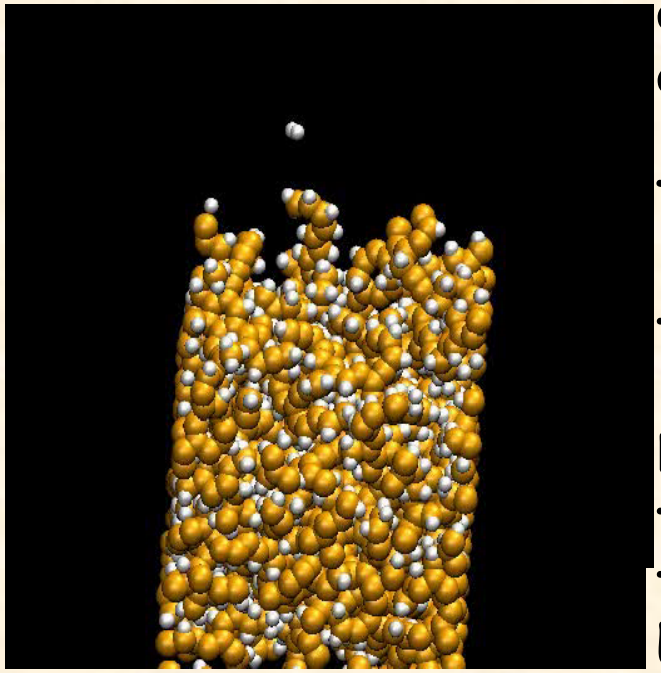
DEMO (> 2030?):

- Steady-state, power flux ~ 10 MW/m^2
- Hot walls (>600 C)
- Refractory metals
- Neutron irradiation 14.1 MeV (~ 100 dpa)

Parameter range inaccessible in present devices

☞ **valid extrapolation needed!**

What does flux of 10^{25} particles/m^2s mean?



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

The flux is 0.01 particle/nm^2ns
1)1 particle hits the interface surface of the cell each 100 ps.

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

In effect interaction of an impact particle with nanosize functionalized macromolecule
News is that each particle will change the surface for the subsequent impact: Here comes the synergy!

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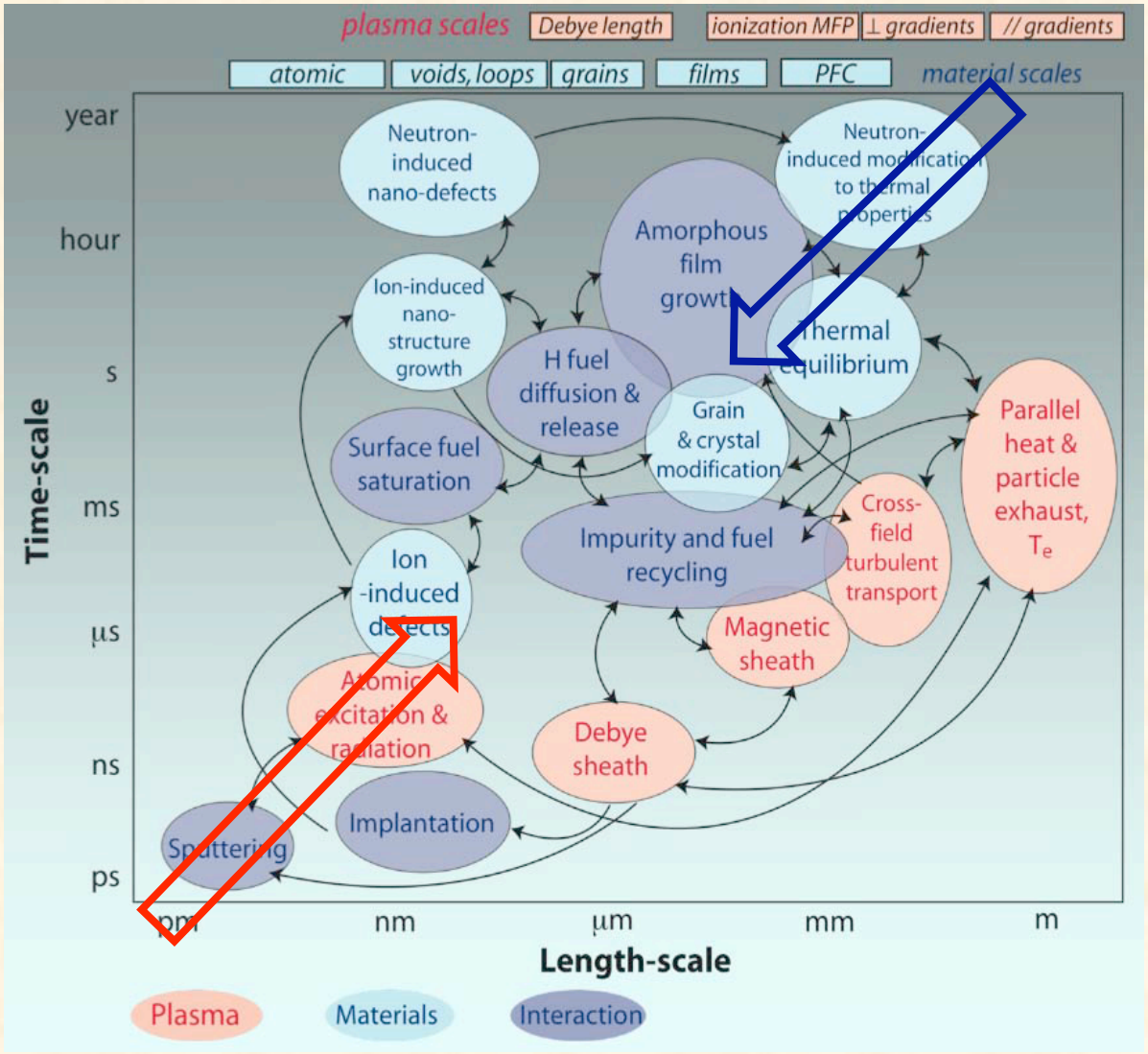
PMI: multi-scale, multi-dimensional, multi-mechanism problem

Seek quasi-equilibrium: (burning plasma ⇔ wall)

Advances in theory &computing enable bottom→up approach in contrast to top→down



Courtesy of J.P. Allain

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

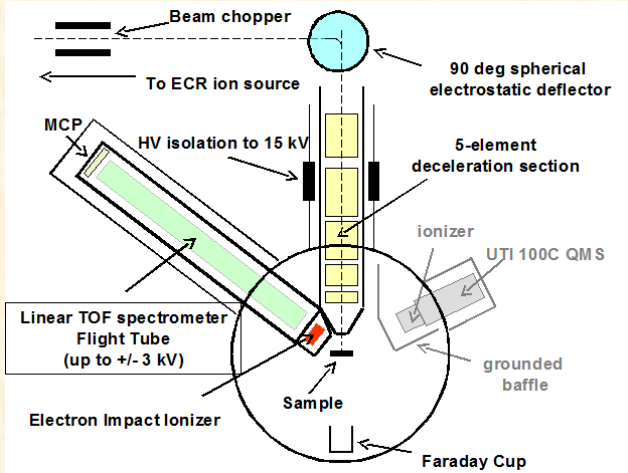
The traditional trial-and-error approach to PMI for future fusion devices by successively refitting the walls of toroidal plasma devices with different materials and component designs is becoming prohibitively costly.

PMI is key fusion research area and is getting a strong momentum

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."

2009: DOE Fusion Strategic Workshops recommendations
Decode and advance the science and technology of plasma-surface interactions.
Develop improved power handling through engineering innovation.
Establishment of new PMI facilities and programs

Beam-surface exp't: precision control of projectiles & targets . . .



- Control of impact energy & angle.
- Incident flux up to 10^{19} m^{-2} s^{-1}
- Clean, well-characterized surfaces, pb~10^{-10} torr
- Temperature control of target
- Absolute yields of interaction products
- Direct line of sight for diagnostics (TOF, etc.)

ORNL: F.W. Meyer,

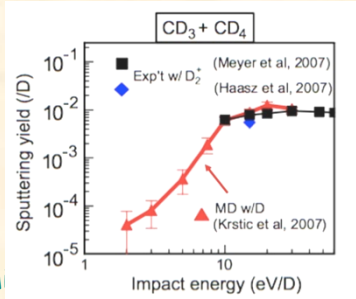
. . . enabled development & validation of MD approach

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

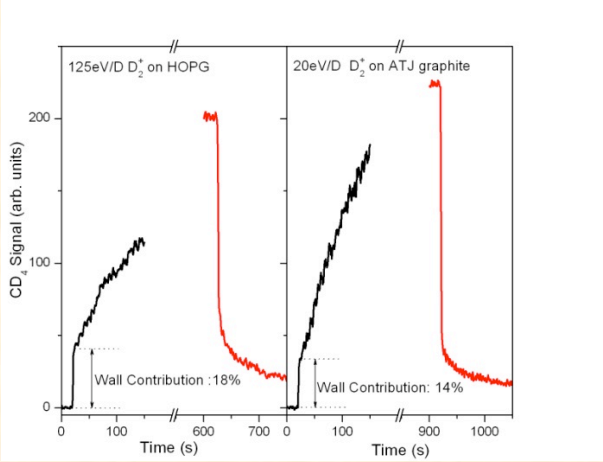
Krstic & Meyer, 2007



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

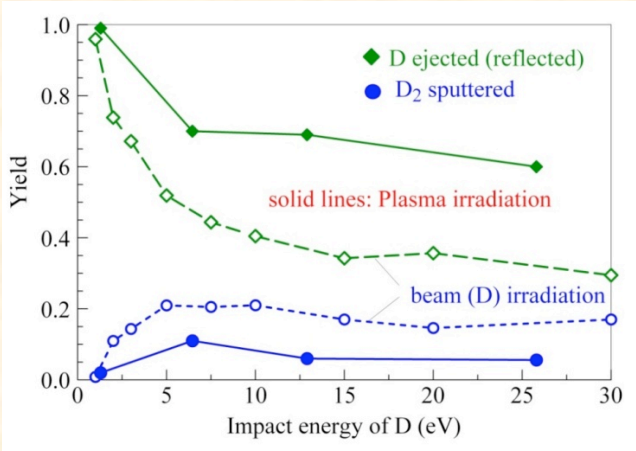
Deuterium impact of carbon

Methane sputtering requires H loading of the surface



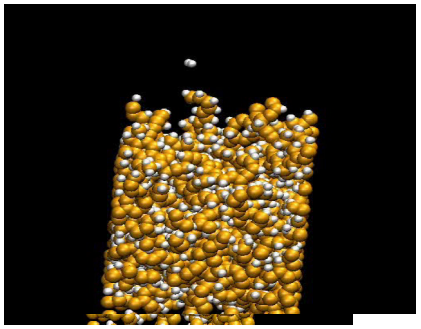
F. Meyer, 2007

Plasma irradiation results in a different surface

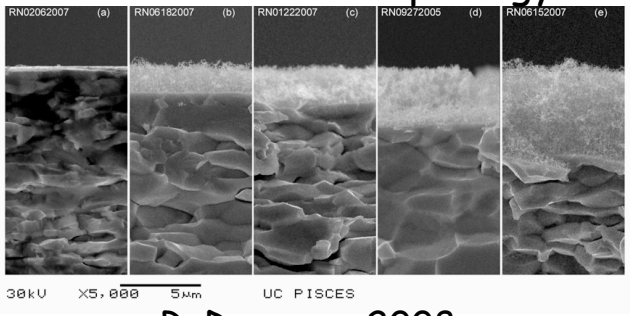


P. Krstic, 2008

Chemical sputtering of hydrocarbons



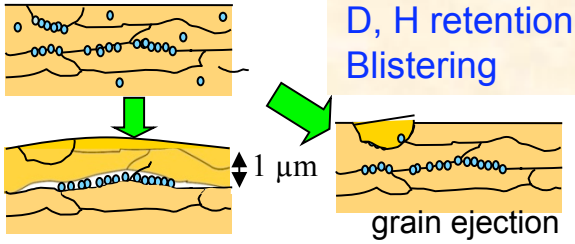
Surface morphology



R. Doerner, 2008

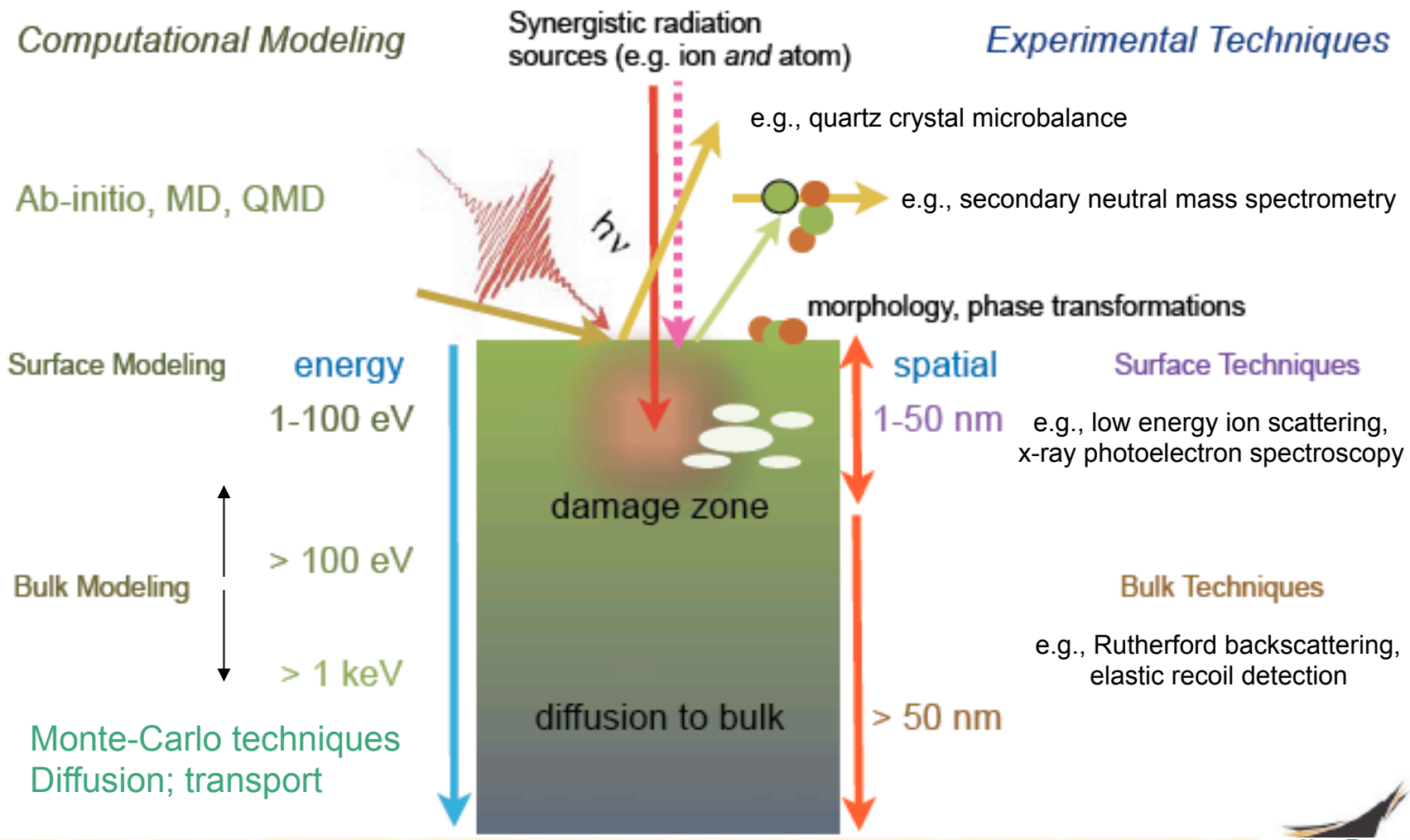
Nano-fuzz on W irradiated with He

Sub-surface structure (W)

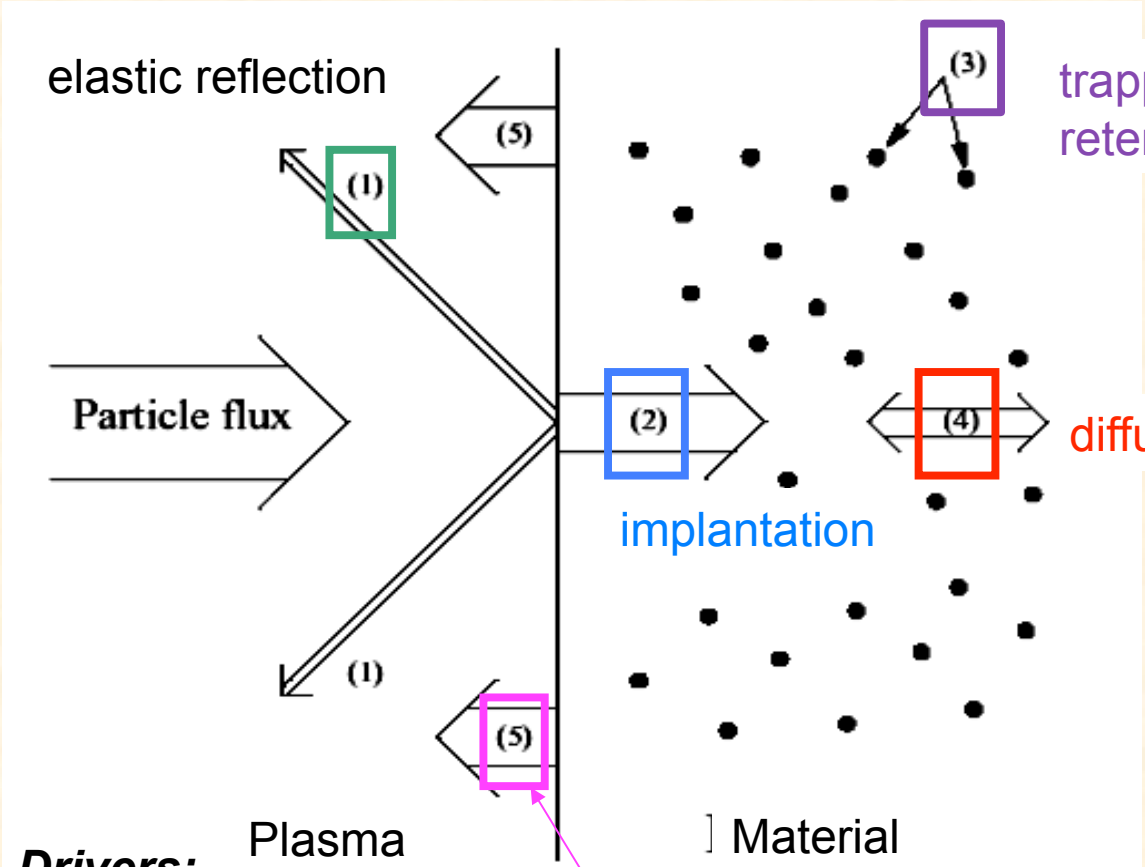


D, H retention
Blistering

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



PMI has many fundamental processes & synergies



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

re-emission &
sputtering &
chemistry

Damage Effects:
Vacancies, bubbles, blisters,
dislocations, voids, neutrons?

Give rise to synergistic effects

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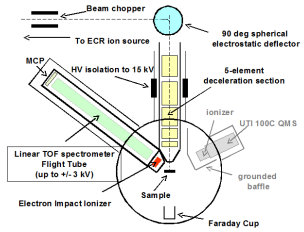
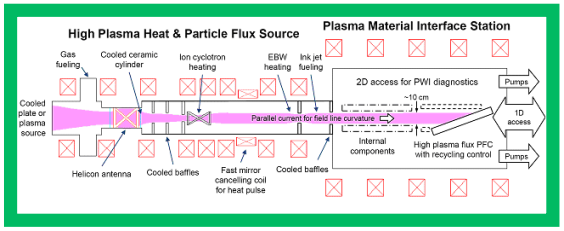
Full integration of the three main branches of the PMI research is hoped!

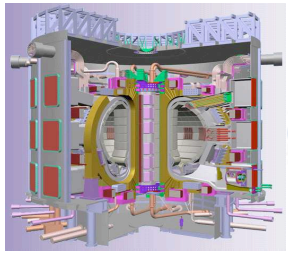
Beam-surface experiments:
Prepared beam & target

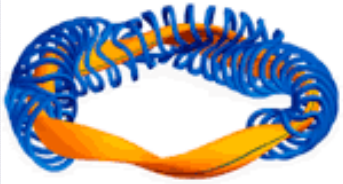


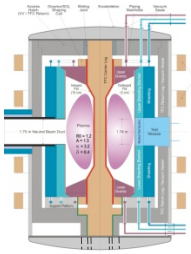
High-flux linear PMI experiment:
Well-diagnosed plasma & target



Toroidal confinement experiments







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

Potential models
Quantum-classical MD

Increases in computational power

MD and MC with plasma synergy

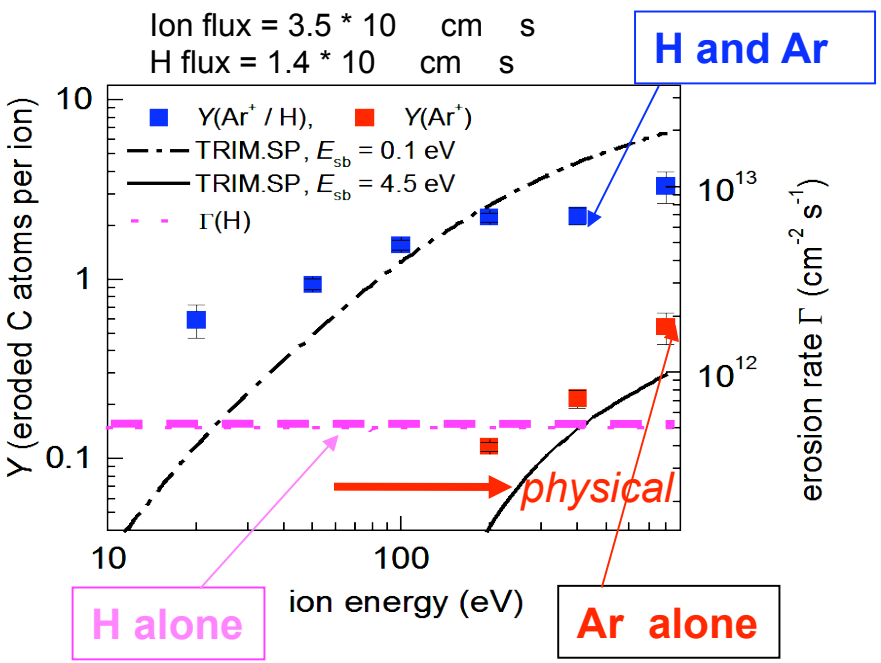
PMI Design & Qualification

ITER, DEMO

Understanding synergies of species

Experiments with Ar+ and H beams:

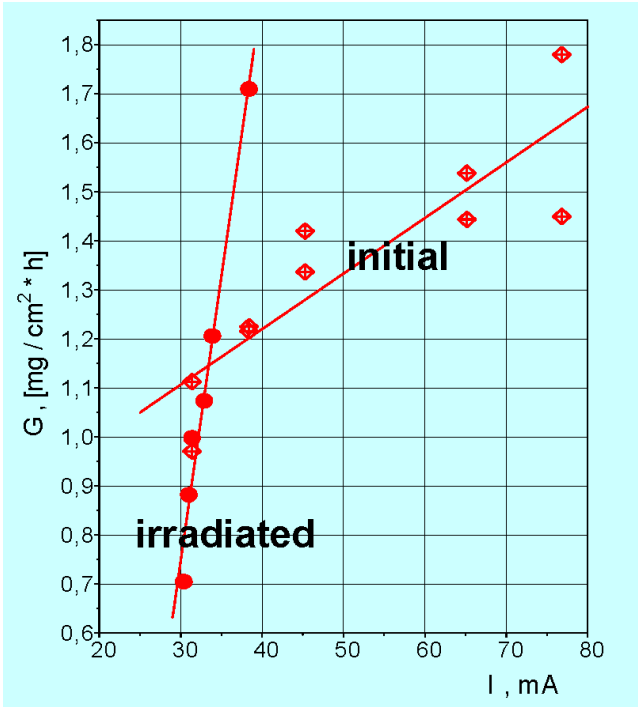
- Sputtering = (chemical) + (physical)
- Surface preparation by H impact for chemical sputtering
- Impurity atoms in plasma are efficient precursors for erosion
- PM processes very dependent on inventory of H in the material



Hopf & von Keudell, 2003

Exposure of pyrolytic graphite to 5 MeV C+ beam simulates neutron damage:

- more nucleation⇒ enhanced erosion
- sites for H retention
- increased HC density?
- increased ejection probability?



B.I. Khripunov et al. 2009

The most complex PSI: Chemical sputtering

Our basic simulation cell:~ 2500 atoms)

***Bombardment** by ions, atoms, molecules*

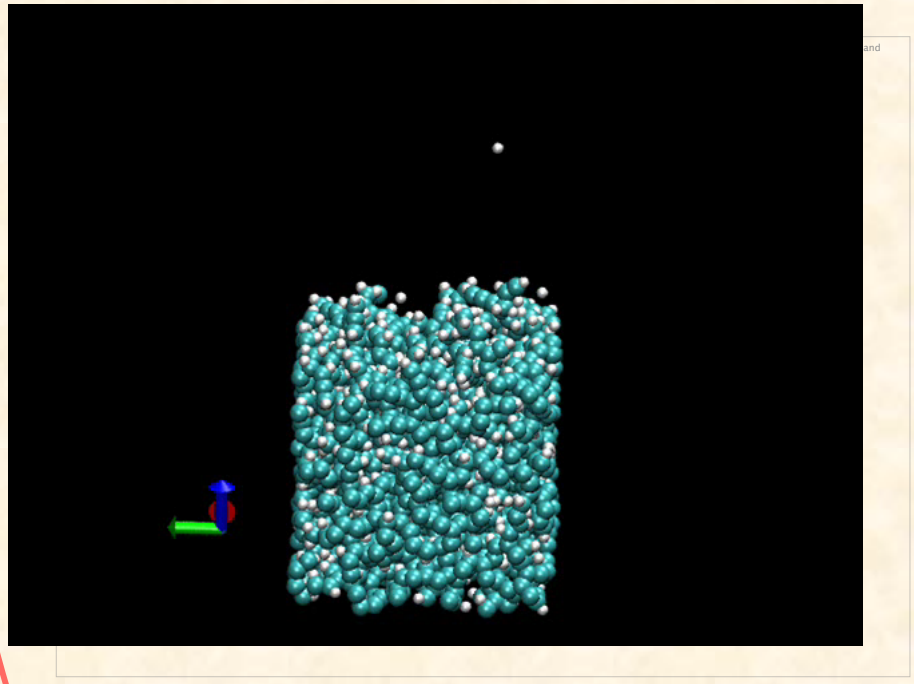
***Chemical reactions** inside the surface (Breaking C-C bond, H pacifies bonds)*

***Produced volatile particles** diffuse, or more likely travel through voids*

***Desorbed** into the gas phase*

Some promptly re-deposited, Most released into the plasma

Released particles transported with plasma, changed, deposited to some other PFW



D atom (20 eV) on supersaturated a-C:H

COULD BE MULTISCALE AT HIGH IMPACT ENERGIES

- OPEN BONDS OF C ARE PACIFIED BY H, HYBRIDIZED INTO SP^3, SP^2,

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Function of :

PROJECTILE

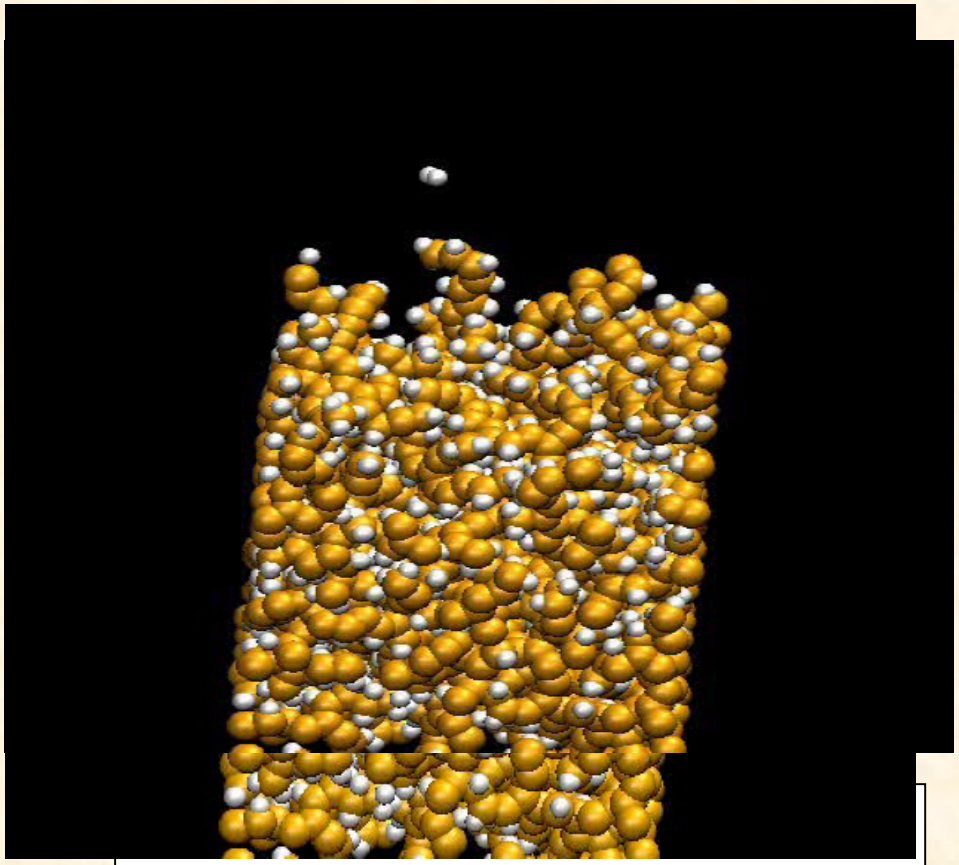
-Type (H, H2, Ar, N, He)
- Impinging projectile energy (1-100 eV), angle
- Internal state of the projectile
- Isotopic effect (D, T)
- Flux density (10 -10 m s)

TARGET

- Surface microstructure
- Crystalline, amorphous a-C, polycrystalline); Doping (Si, B)
- Hydrogenation level (H/C ratio)
- Hybridization level (sp/sp /sp ratio)
- Surface morphology; preparation
- Surface temperature (300-1500K)

- Predefined classical potentials (Brenner, REBO, AIREBO (Stuart))

Limit to < 100 eV (D-D,D-C); <30 eV (C-C)



breaking

internal states of ejectal

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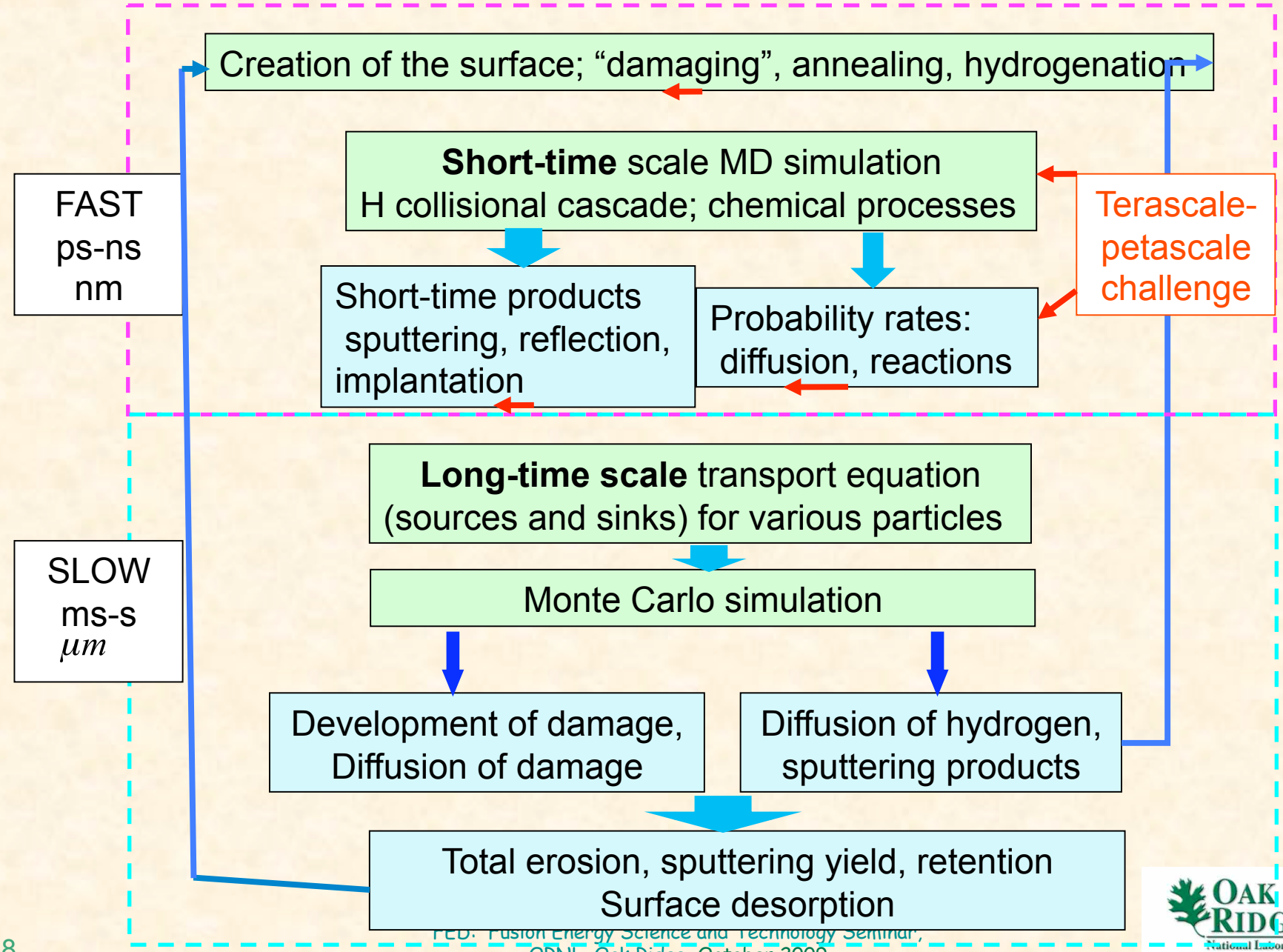
Simulation is computationally intensive and multi-scale



What is molecular dynamics?

- Evolution of a system of particles over time: Duration ~order ps-ns
- Equations of motion are solved for each particle at a series of small time steps (energy conservation) 0.1 fs

$$\mathbf{F} = m\mathbf{a} \quad \mathbf{F} = -\nabla U$$

What is quantum-classical molecular dynamics?

- Key physics input in MD is the inter-atomic potential function

Wide range of techniques for: Potential energy: Modeled, predefined function → Classical MD

- Potential energy is calculated at each time step by solving Schrödinger equation for electrons with adiabatic instantaneous Hamiltonian → Quantum-Classical MD

This is happening now: ORNL Cray XT5 : petaflops (142,000 processors)

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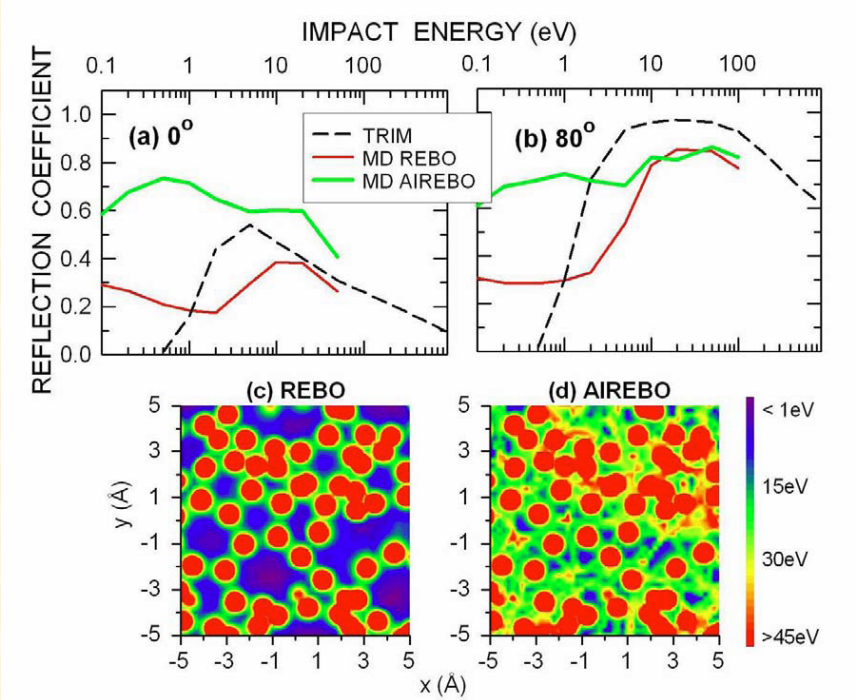
Classical MD is only as good as the interatomic potential model used

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

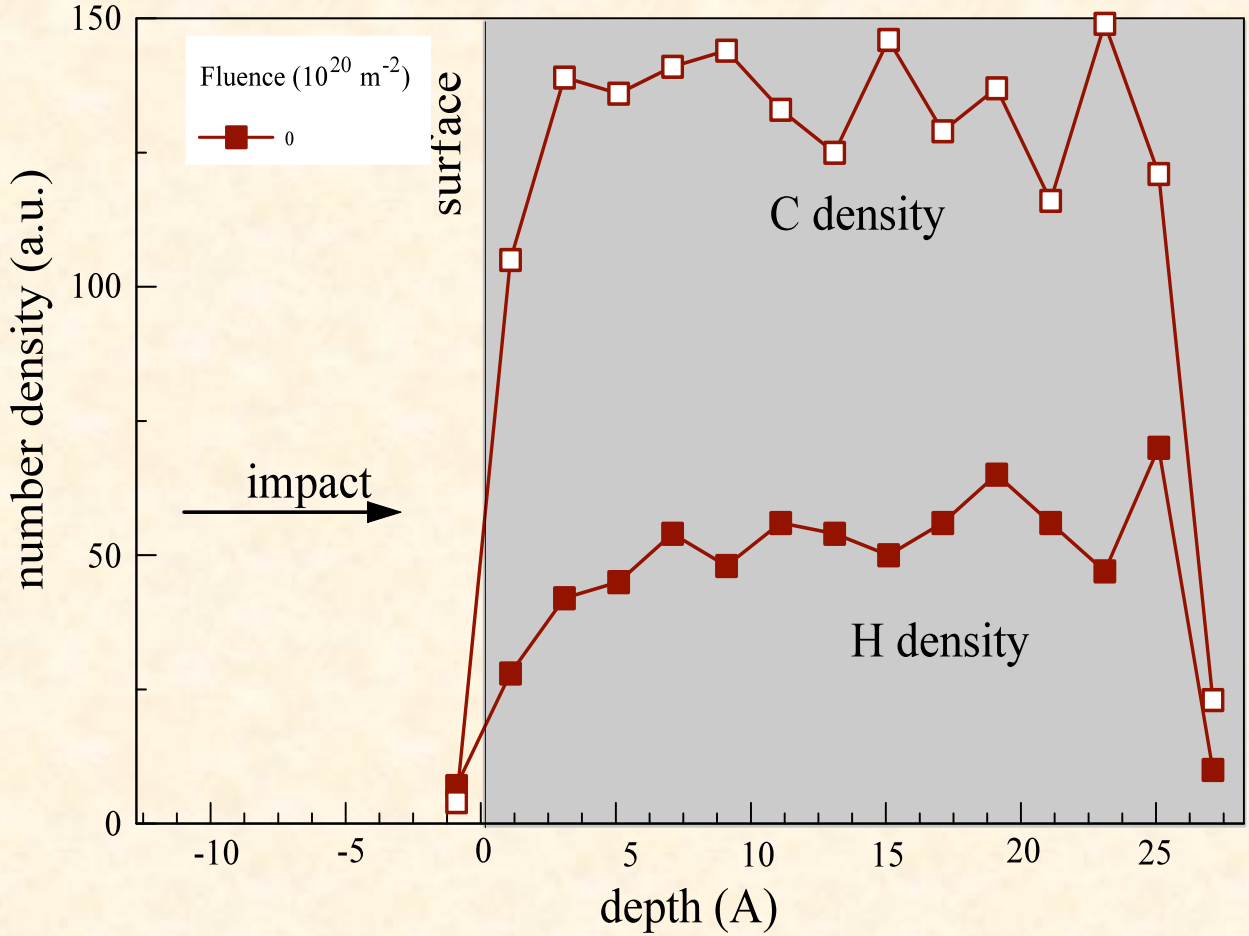
EX: MD calc. of reflection coeff.

- Significant sensitivity to changes in potential model for some processes
- Experimental validation essential to establish credible MD simulation.
- Interatomic potentials for W and Be are less mature than for carbon and require more experimental validation.



Reinhold & Krstic, 2008

Evolution of Density Profile



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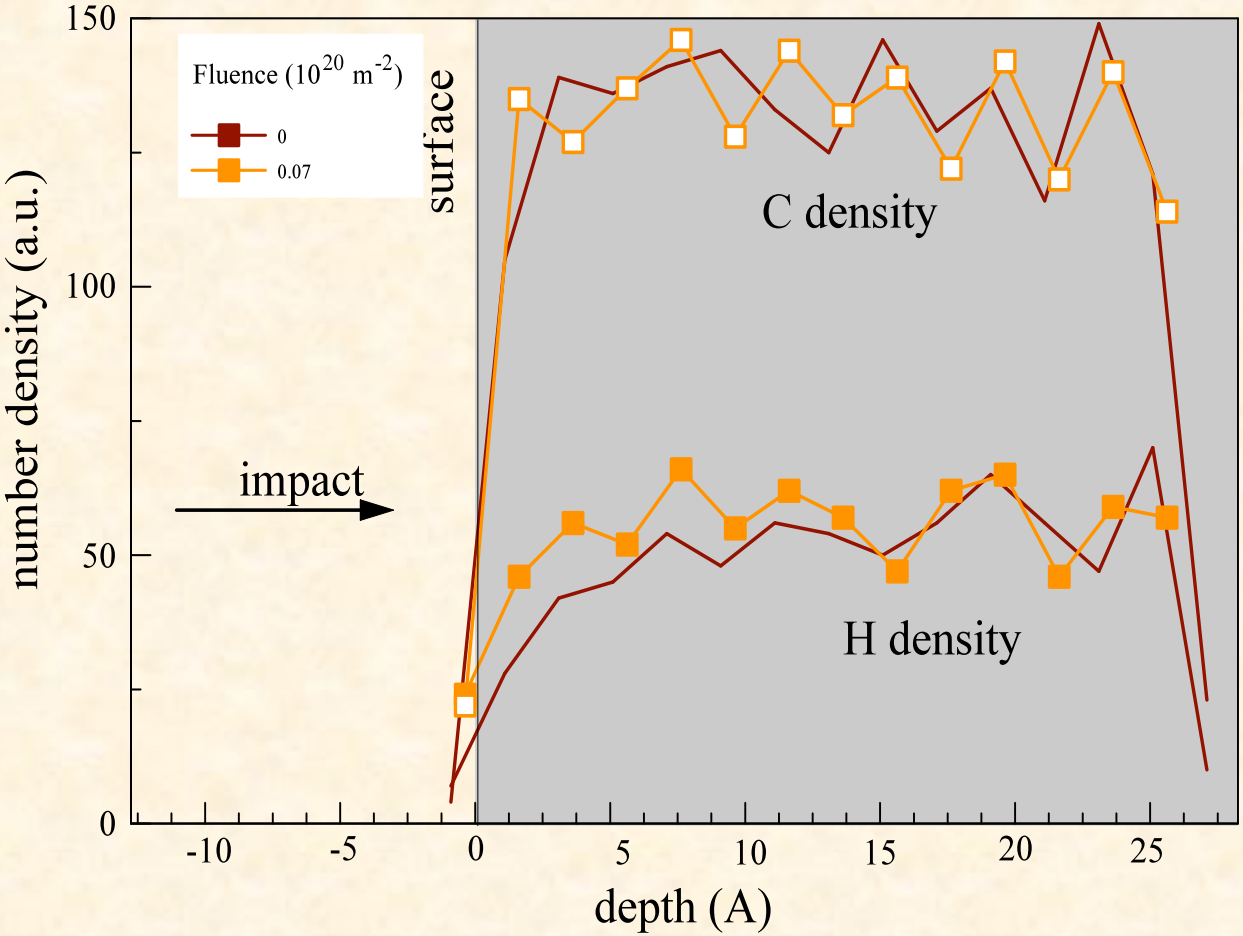

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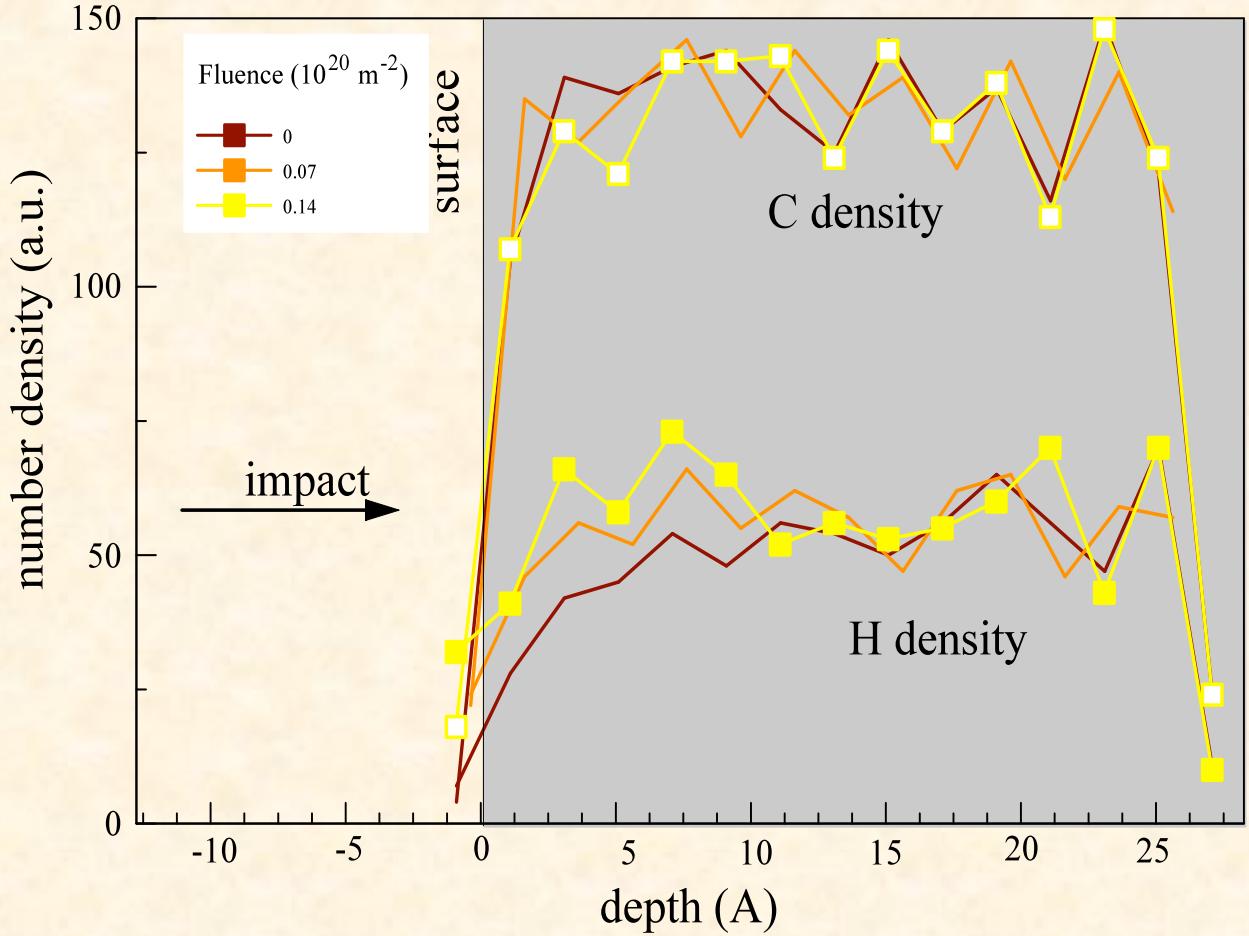

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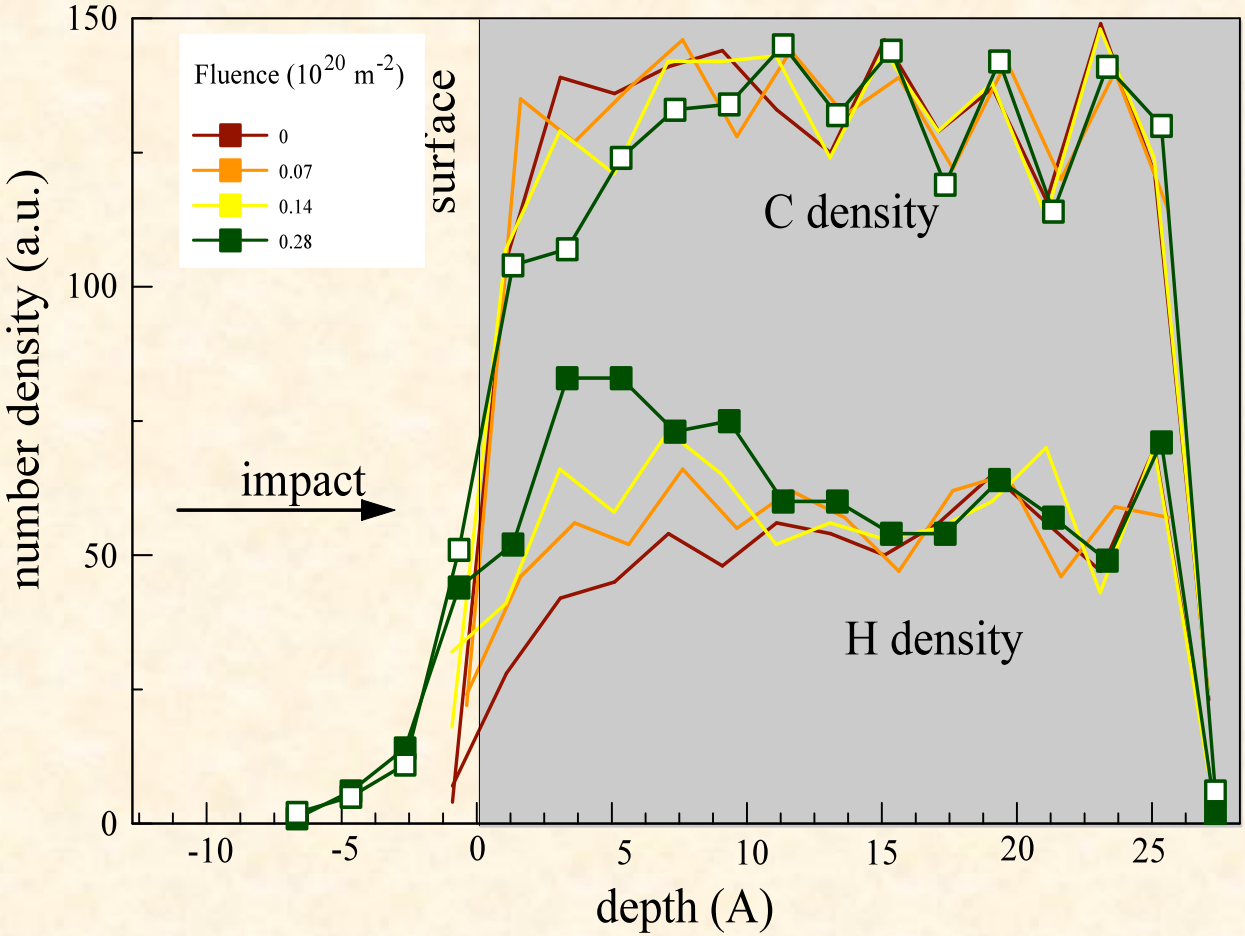

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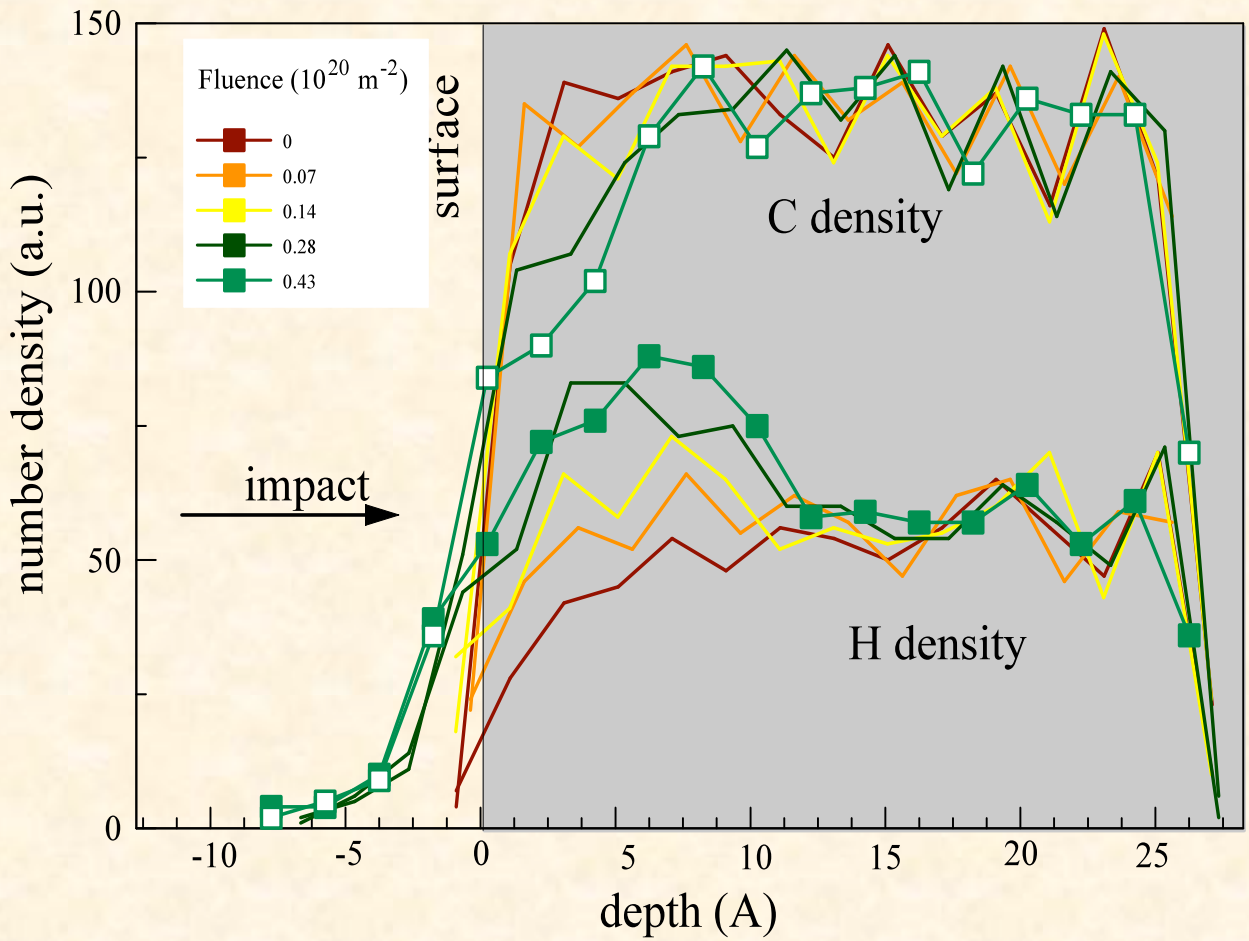

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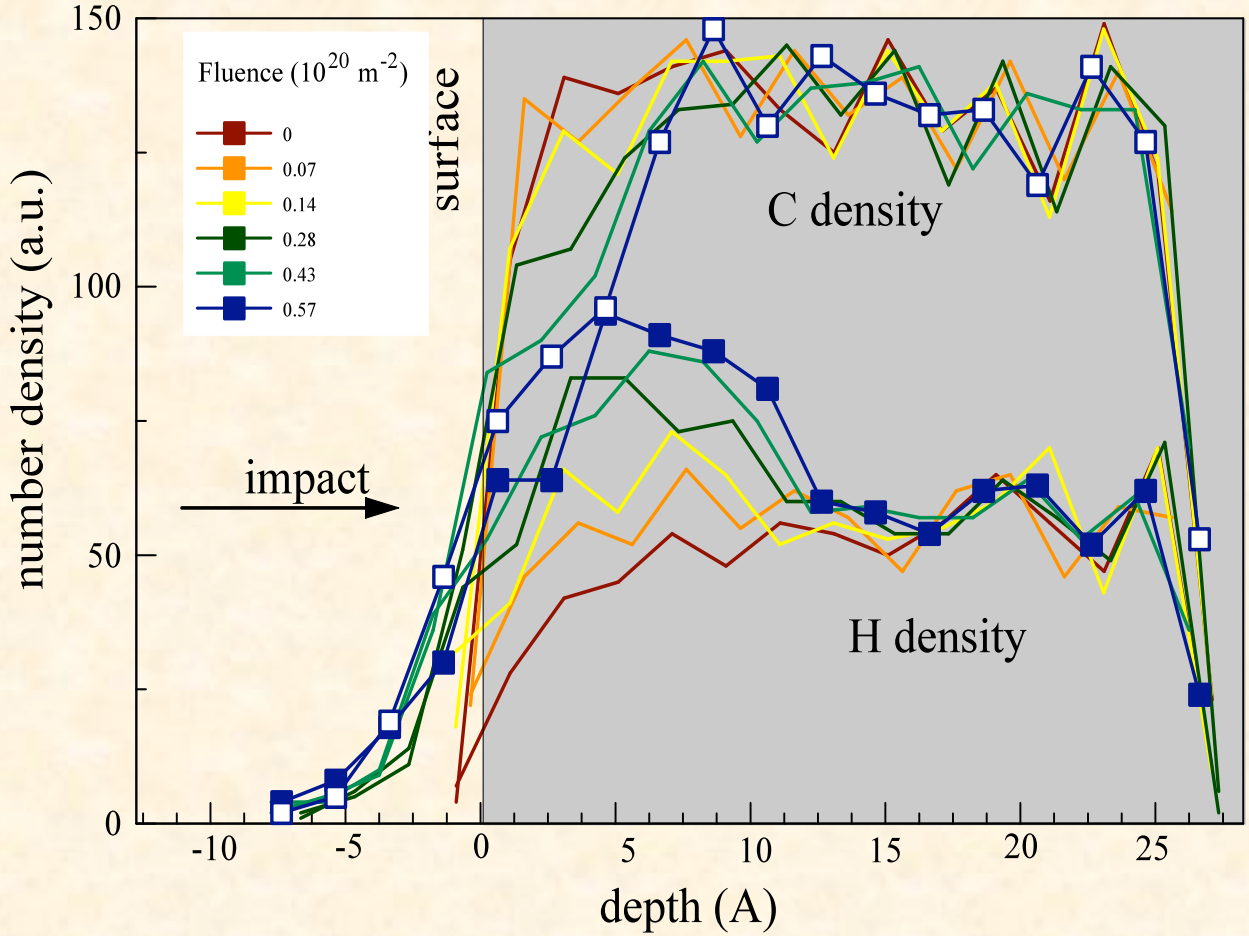

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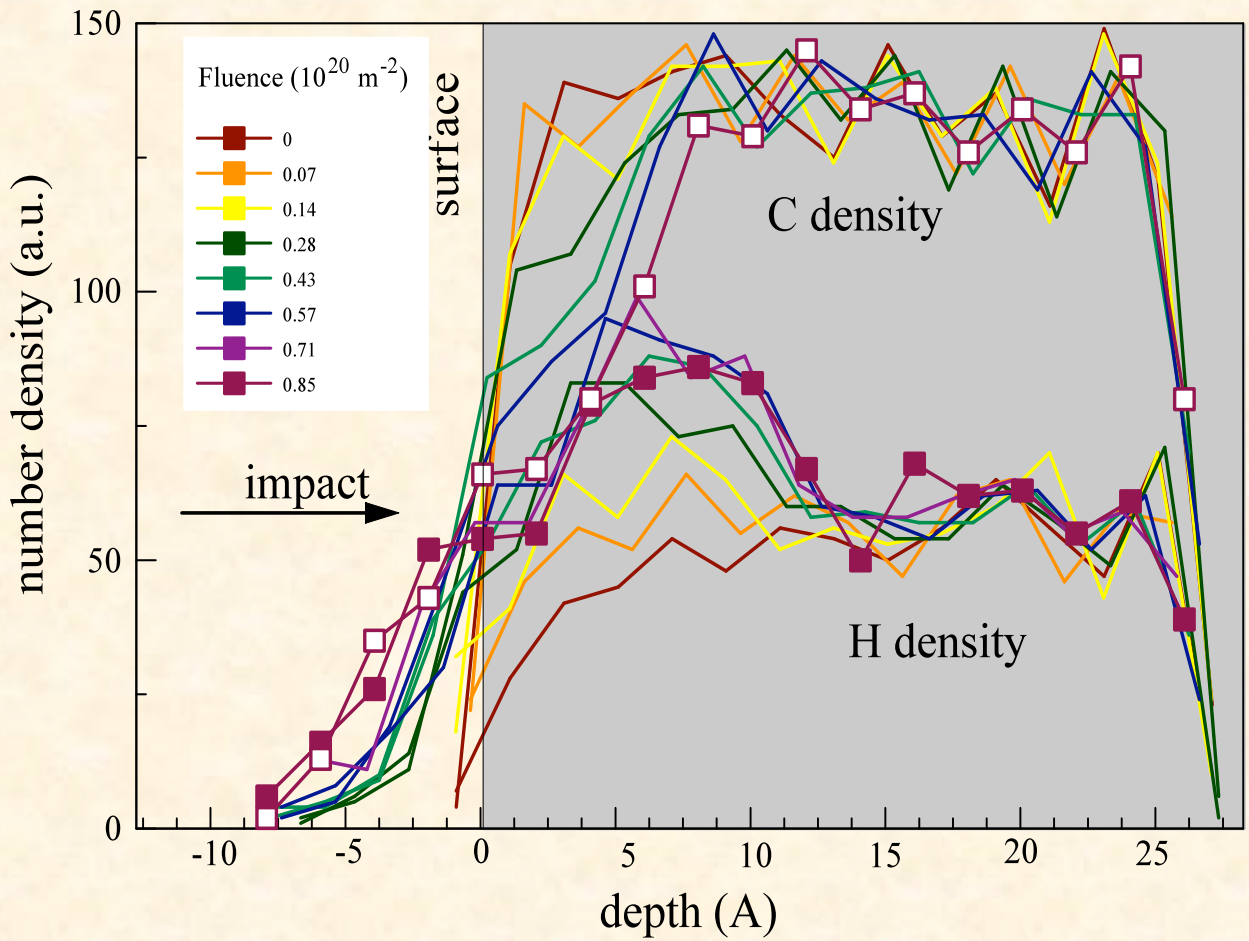

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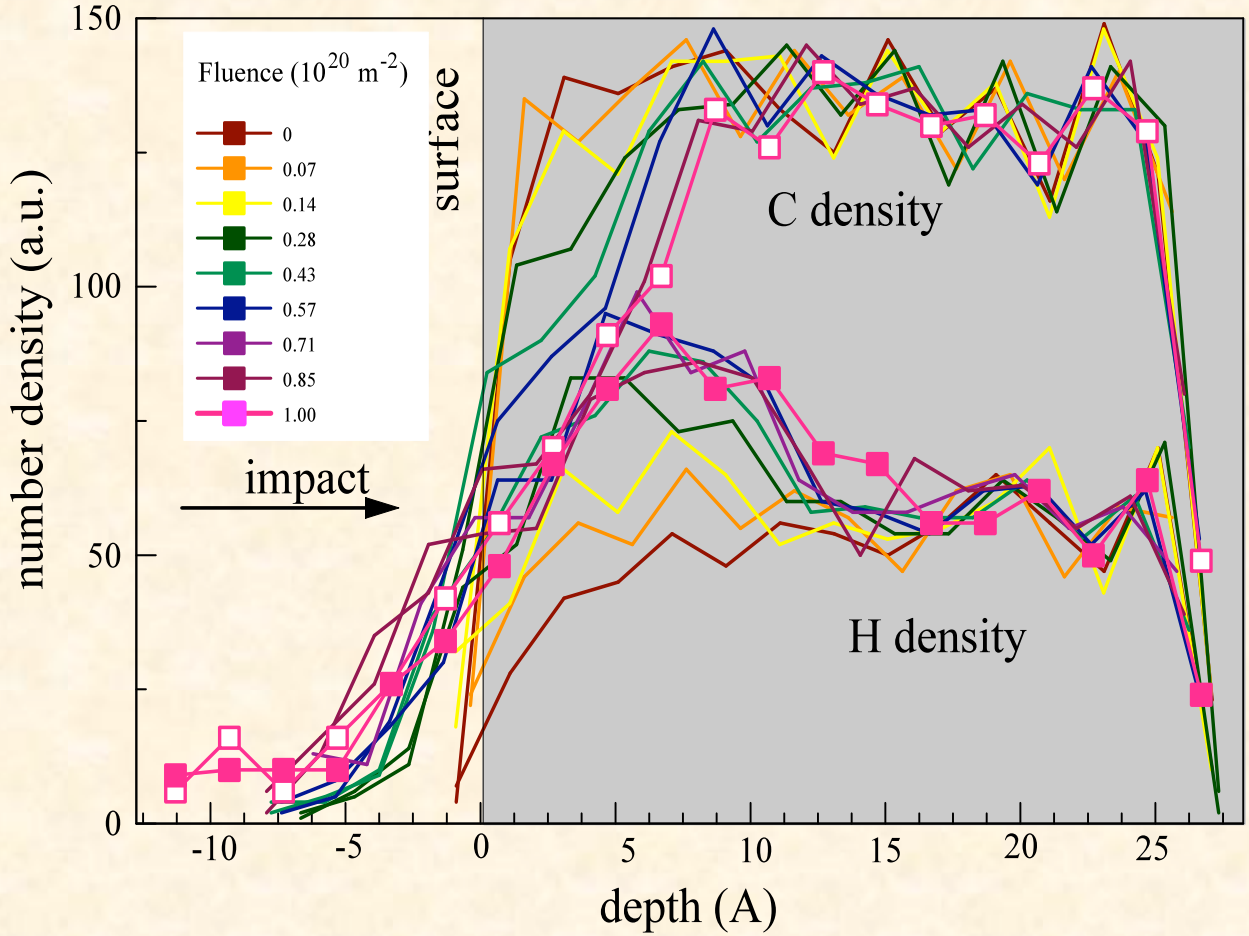

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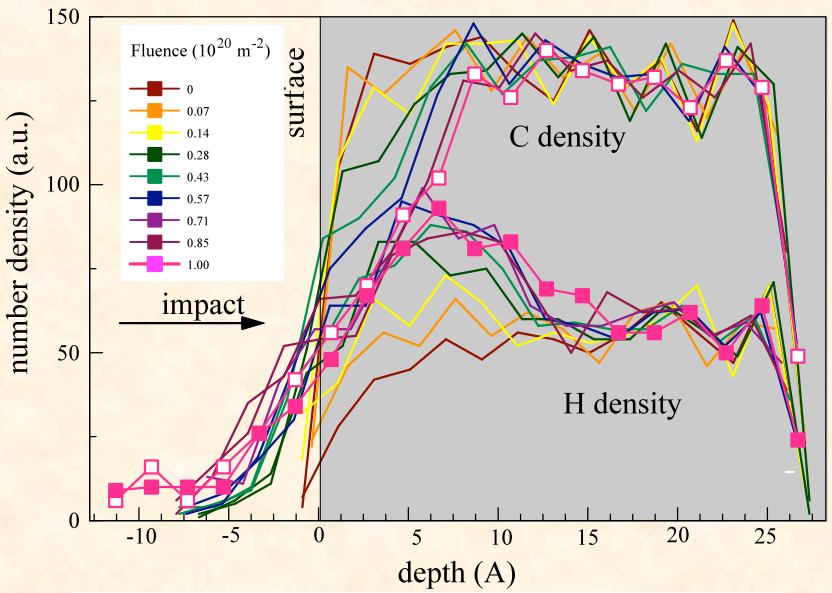

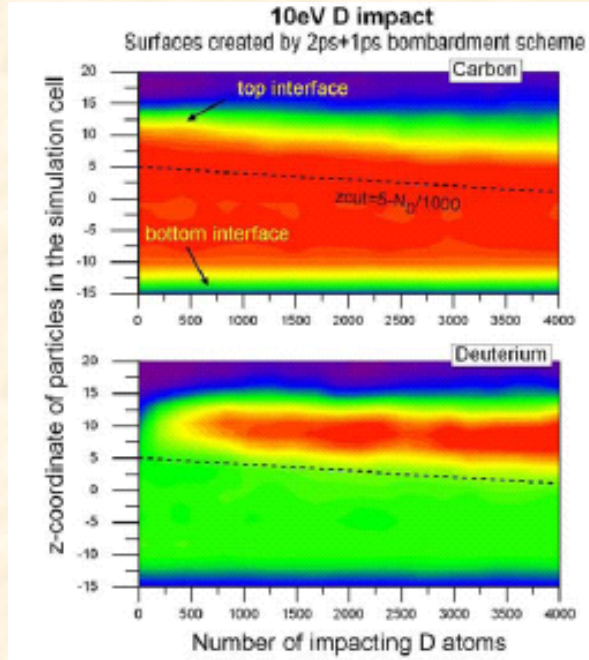

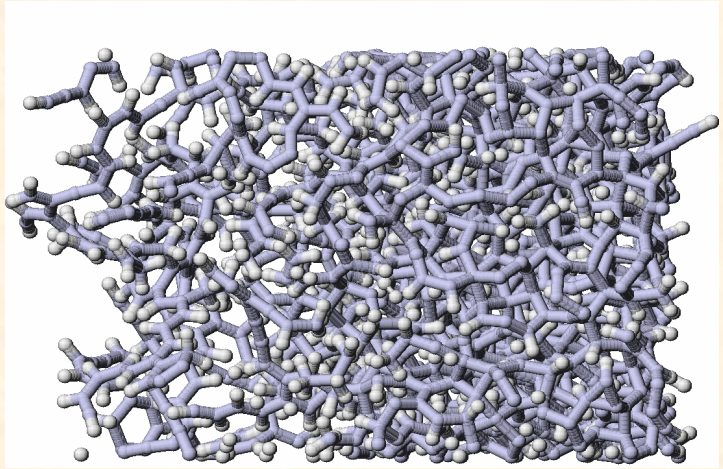

- Surface interface supersaturated with D
- Lower C density at surface
- D/C ~1 at surface
- "Steady state" achieved by fluence of ~ 10^{20} m^{-2}
- Surface depth ~20 Å

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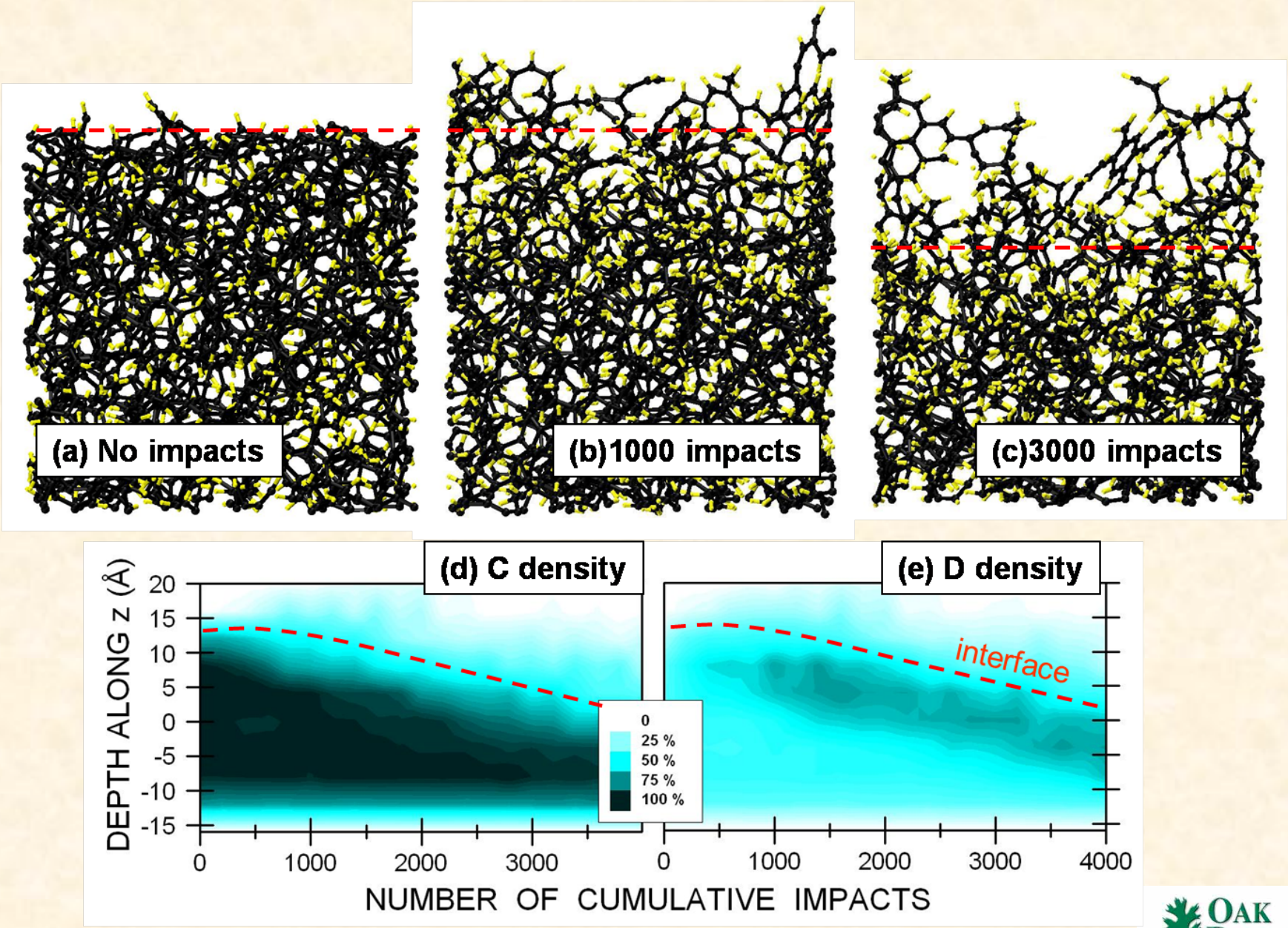
(a) No impacts
(b)1000 impacts
(c)3000 impacts
(d) C density
(e) D density
interface
DEPTH ALONG z (Å)
20
15
10
5
0
-5
-10
-15
0
25 %
50 %
75 %
100 %
0
1000
2000
3000
0
1000
2000
3000
4000
NUMBER OF CUMULATIVE IMPACTS

RESEARCH HIGHLIGHTS

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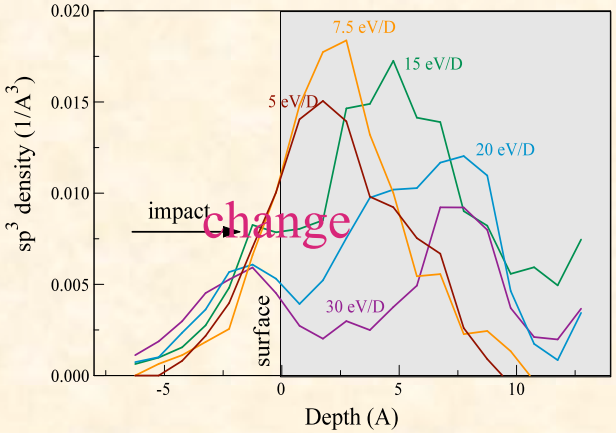
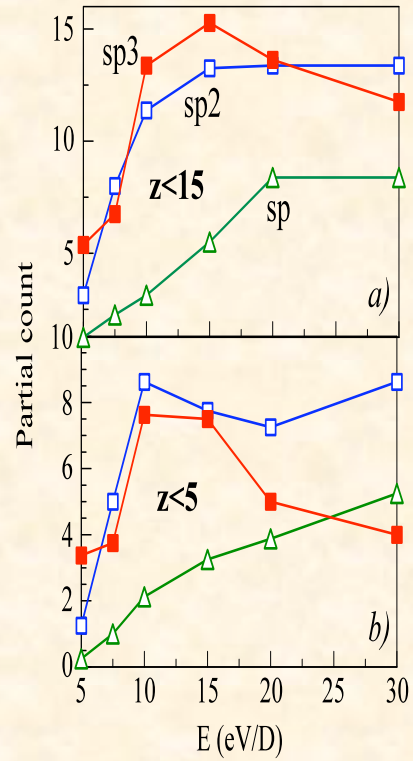
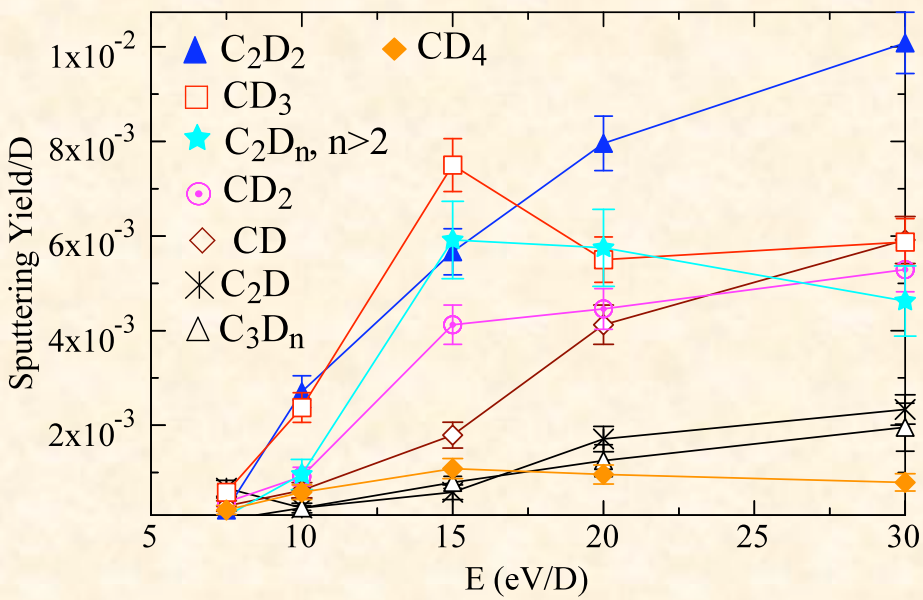
1) Hybridization depth profile, Mechanism of sputtering



C-CD3 : sp3
C-CD2 : sp2
C-CD : sp





Terminal groups bond-braking (TGBB)-subset of swift BB (Salonen)

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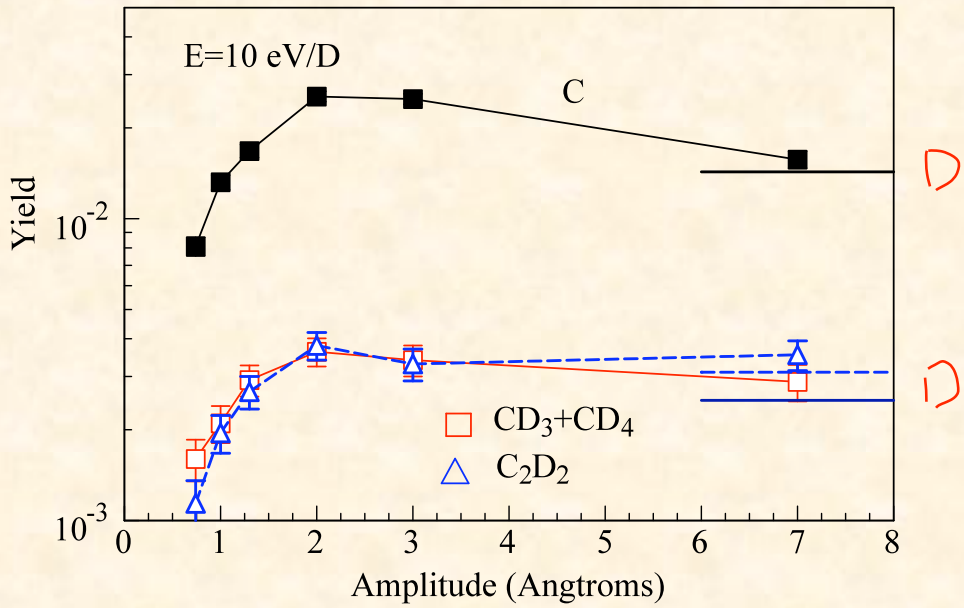
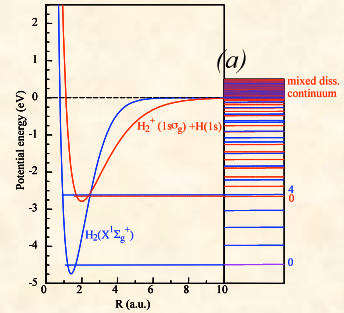
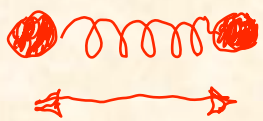
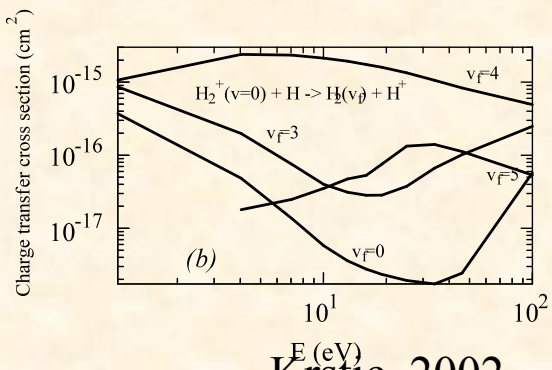
2) Sputtering with (ro)vibrationally excited projectiles









Krstic, 2002

At low impact energies strong influence, most likely due to dissociation balance (4.5 eV)

Neutralization of D2 ions most likely with deposited D

Europhys. Lett. **77**, 33002 (2007).

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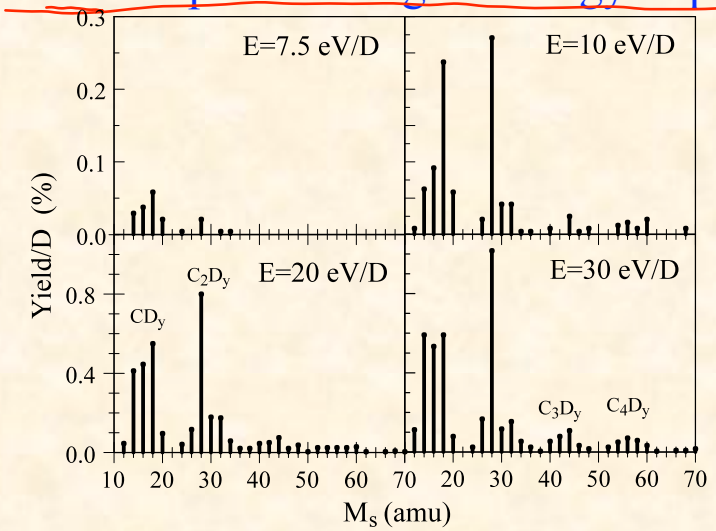
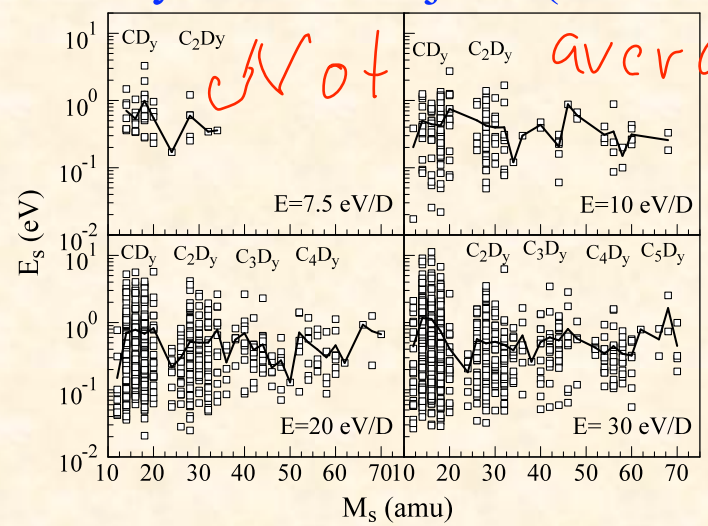
4) Mass/energy spectra of sputtered hydrocarbons
(with excited D2 impact!!!)

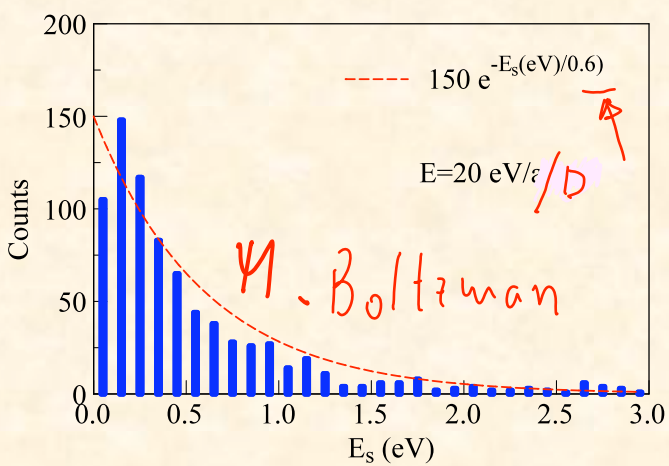
Heavier species at higher energy impact



Hot hydrocarbon ejecta (5-10000K)

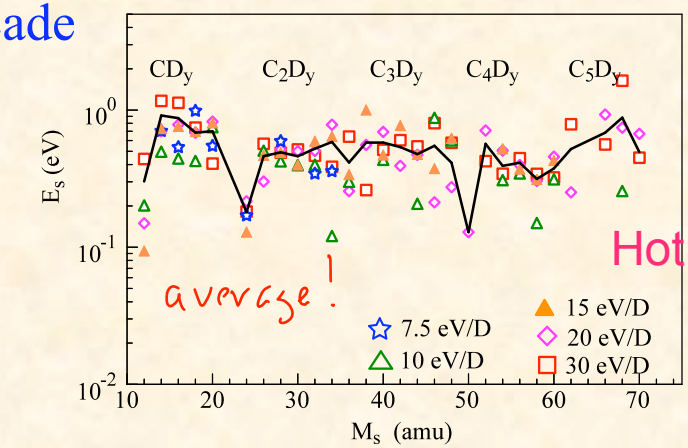


Approximate thermalization along a collision cascade



Kinetic desorption

localized heating!!



Time-of-flight experiment of Vetzke (2002) sees hot hydrocarbons (a few tens of eV)

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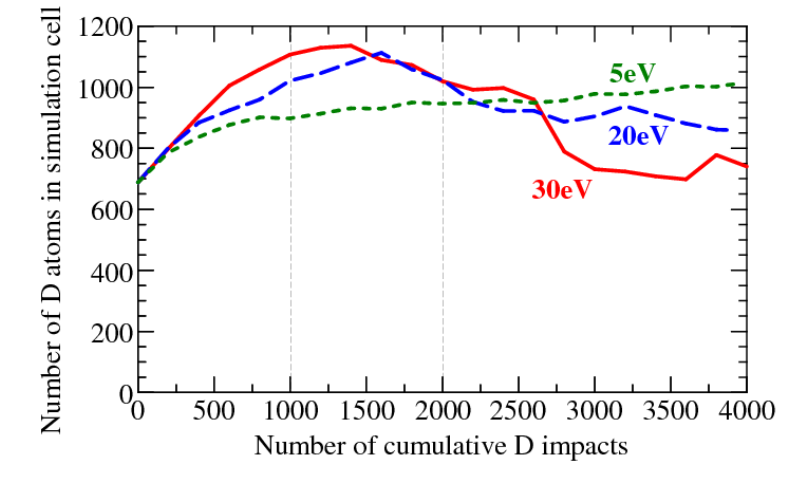
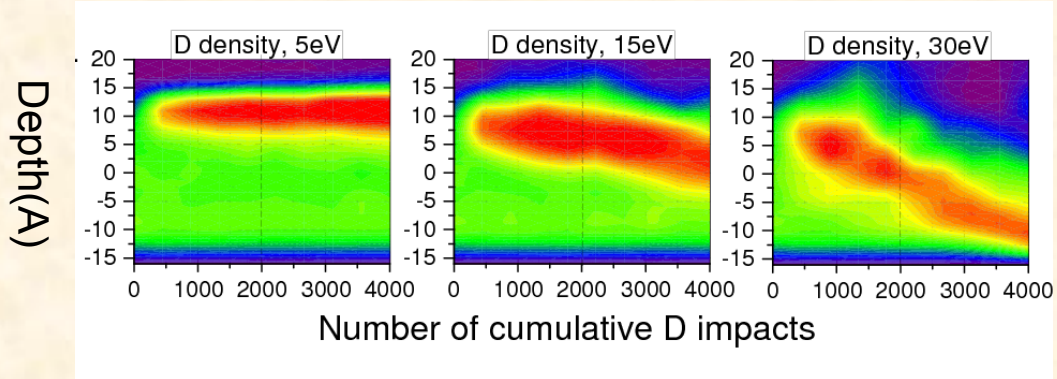
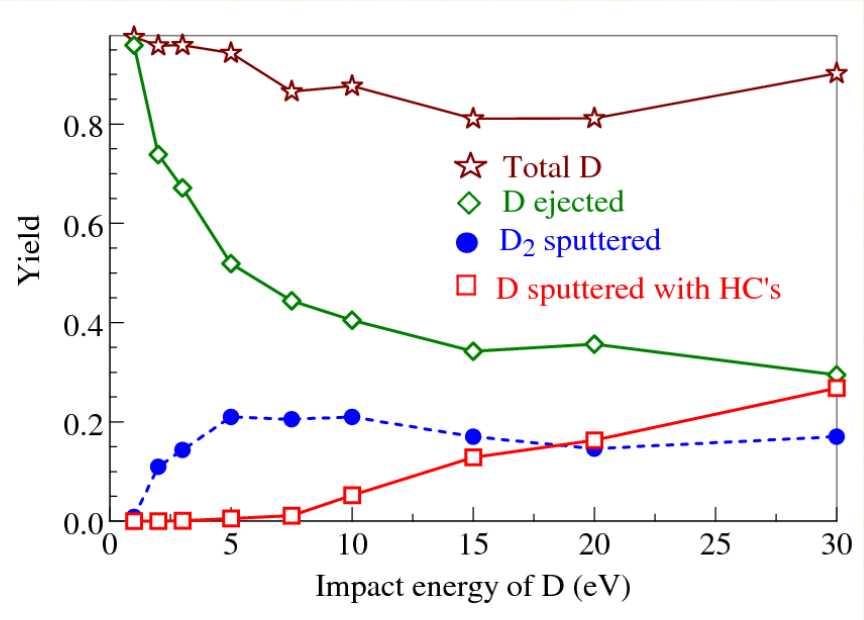
5) Deuterium ejection characteristics upon D impact







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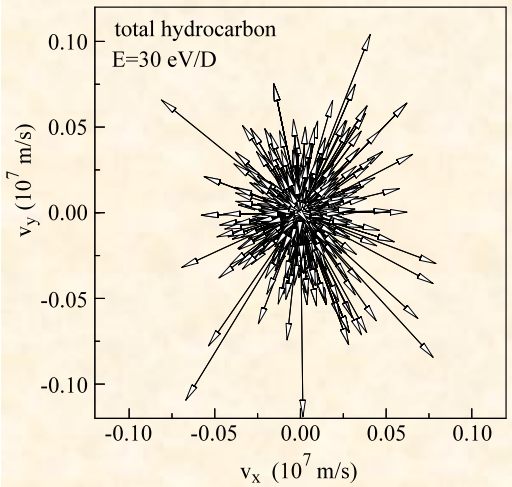
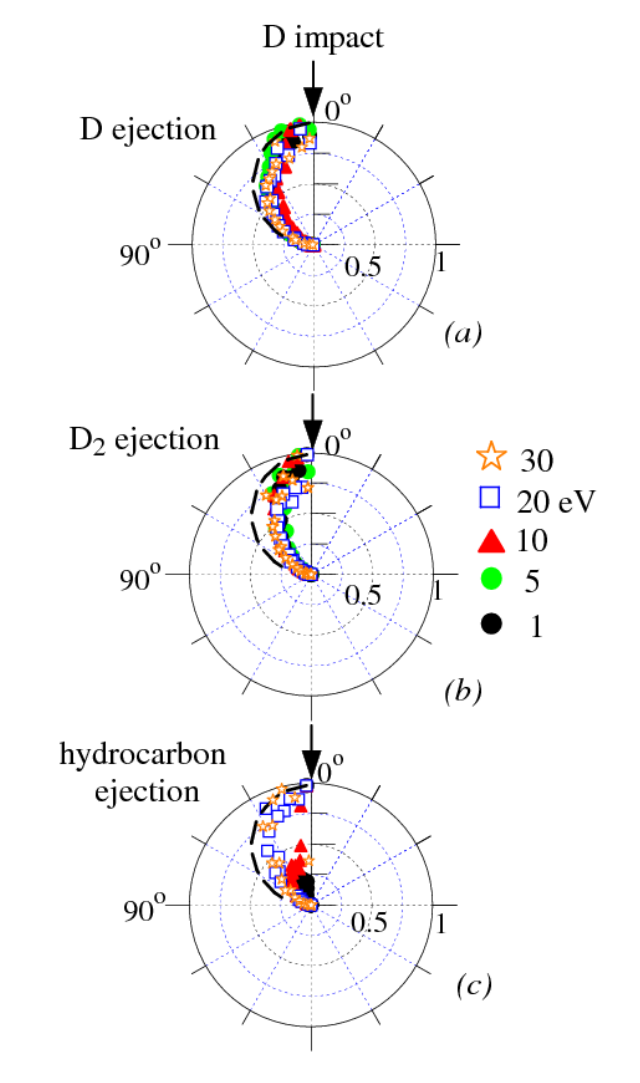
6) ANGULAR DISTRIBUTIONS dn/dΩ

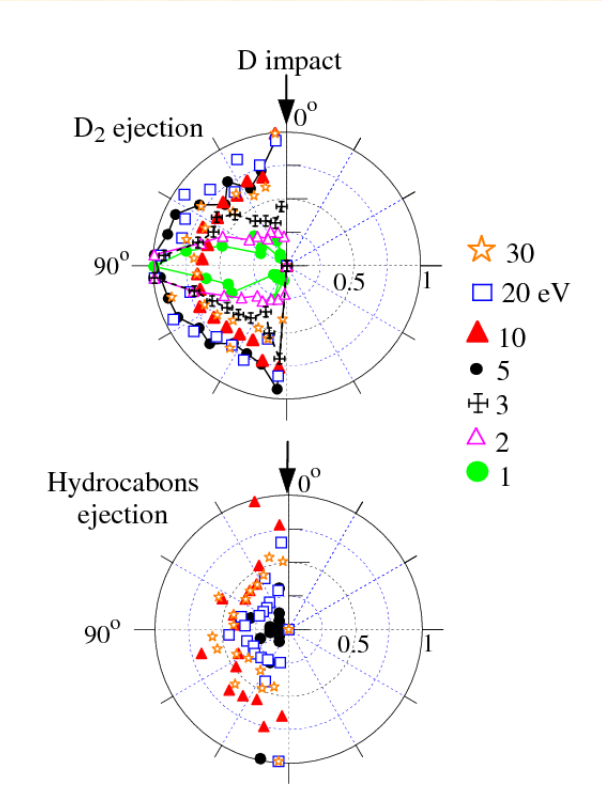


Sum $v_y \simeq 0$

Sum $v_x \simeq 0$



Velocities – cos law



Angular momenta L
sin law or isotropic

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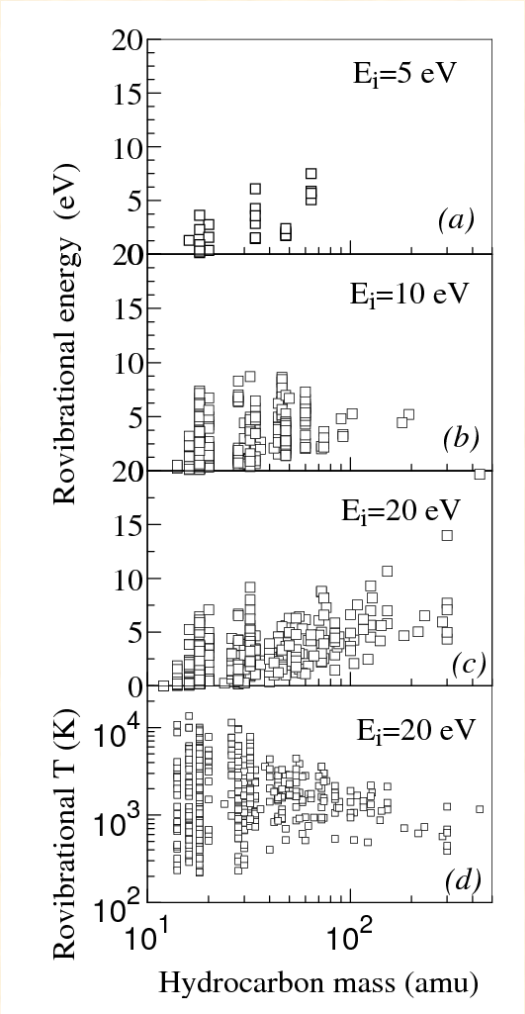
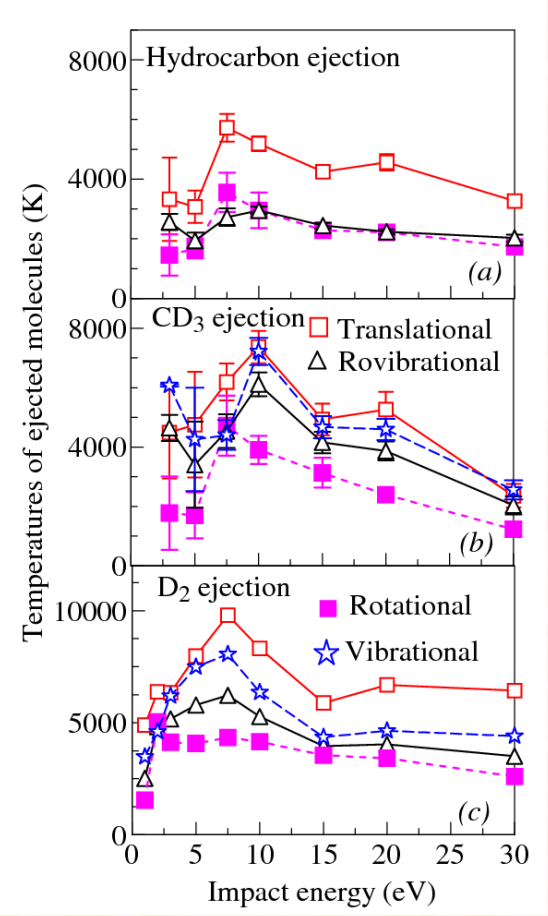
7) Rovibrational energy distributions: Hydrocarbons



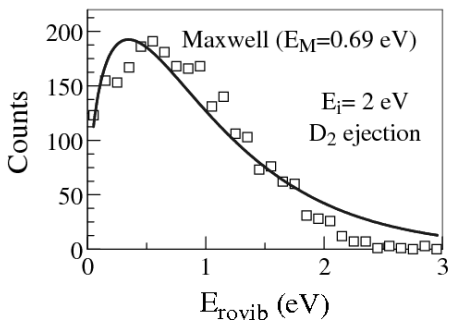
Ejection energy

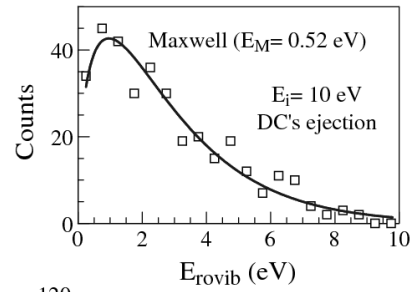


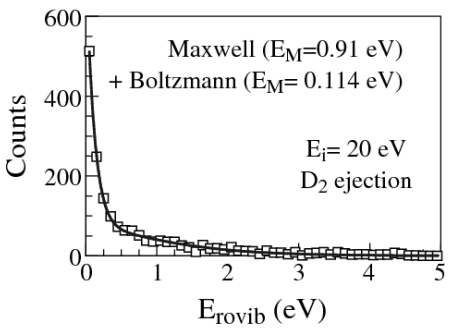
Ejection temperature

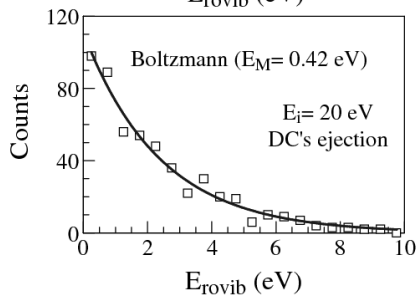
Functions of hydrocarbon mass and impacting D energy

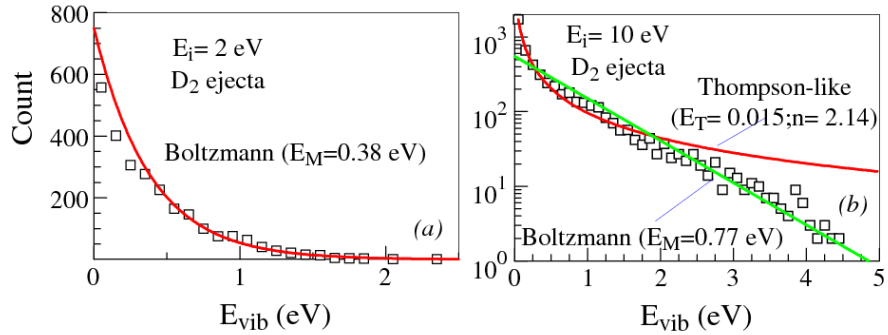
8) Approximate thermalization indicated (rovibrational)



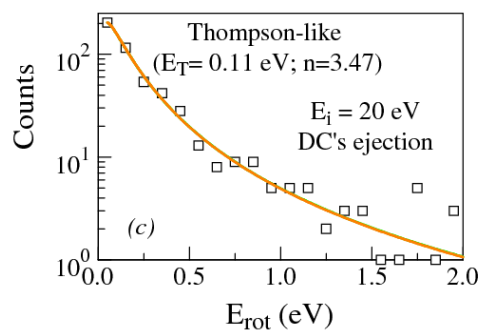








D2 and HC ejecta



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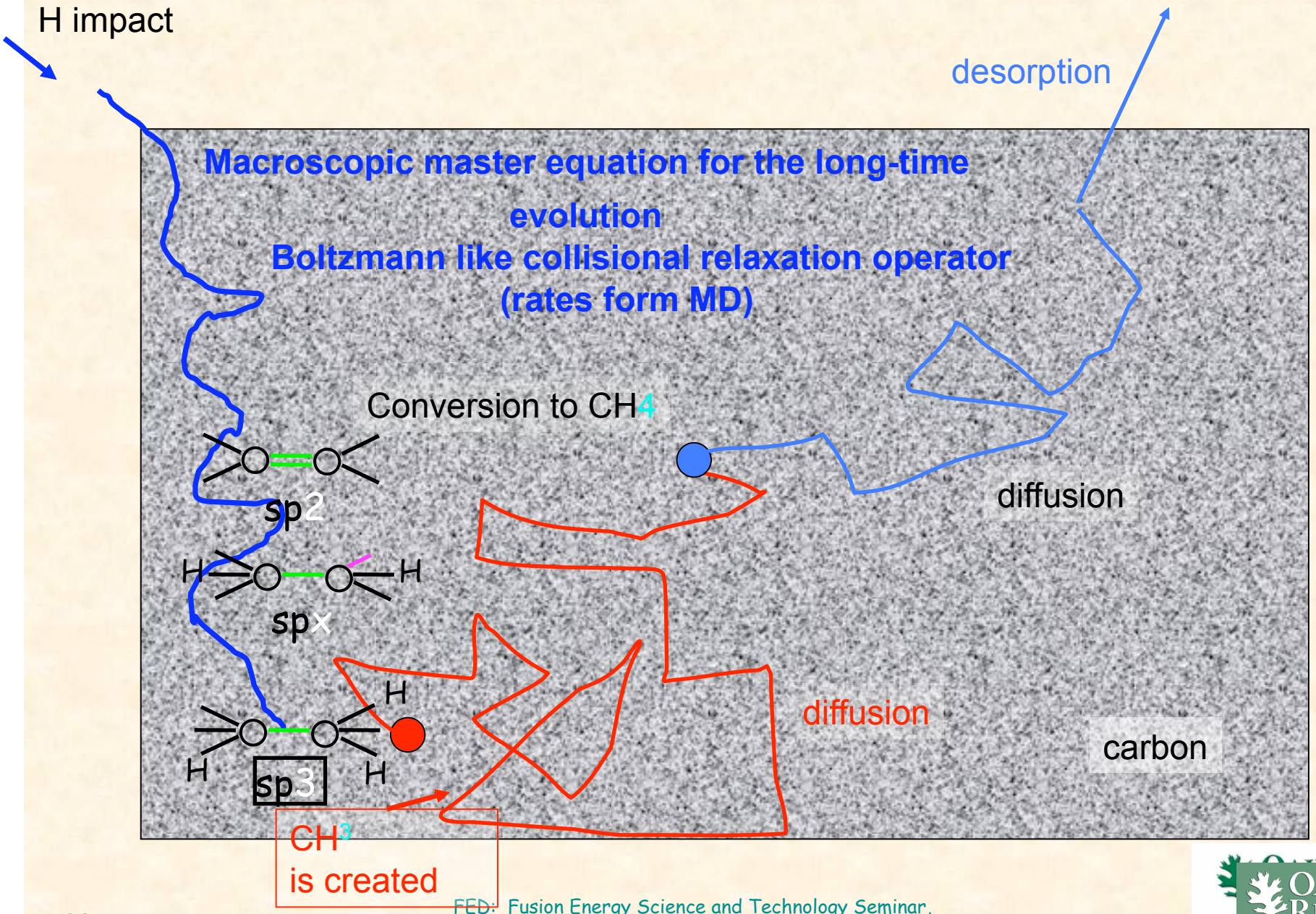
Typical Monte Carlo trajectory approach (ex: a-C:H carbon)



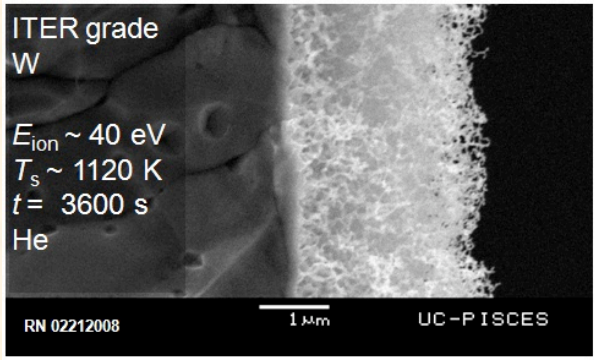
PLASMA IRRADIATION=

Randomization of impact parameters

Synergies in tungsten: dramatic effects in plasma experiments

"Fuzz" nanostructures

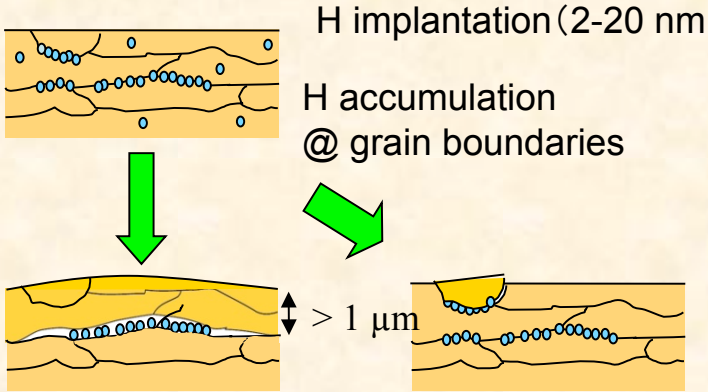
on W irradiated by He
high W temperatures (>1000K)



Baldwin, 2008

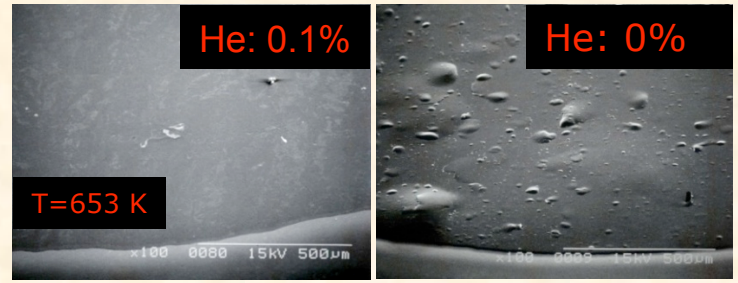
Blistering related to D, H retention

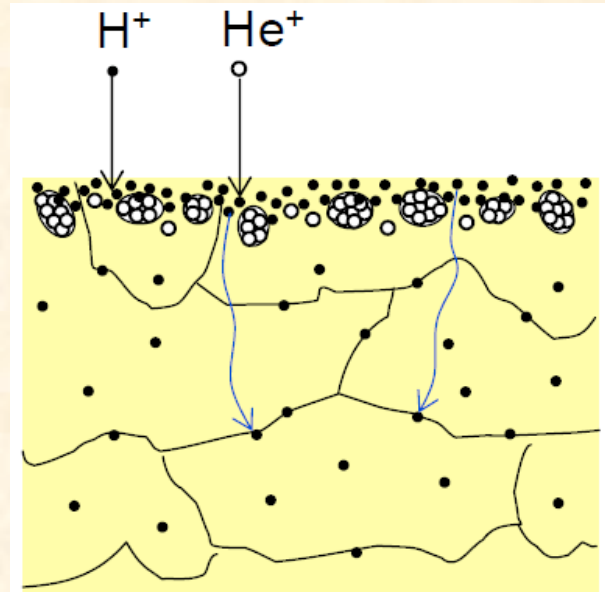
- Sparser for T > 600 K



He suppresses H retention

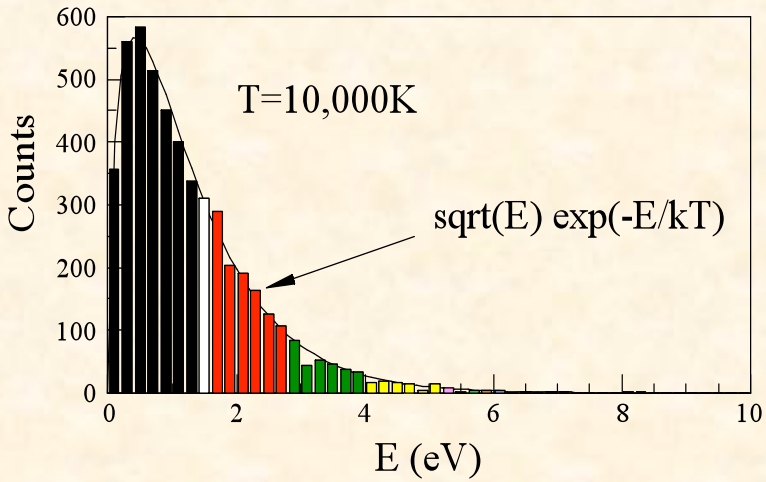
- He penetrates deeper than H
- Strong dependence on energy
- He bubbles: barrier to H diffusion?

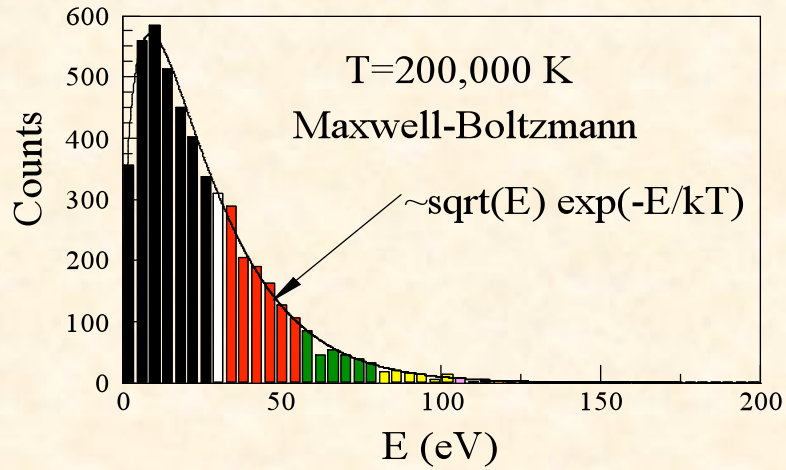


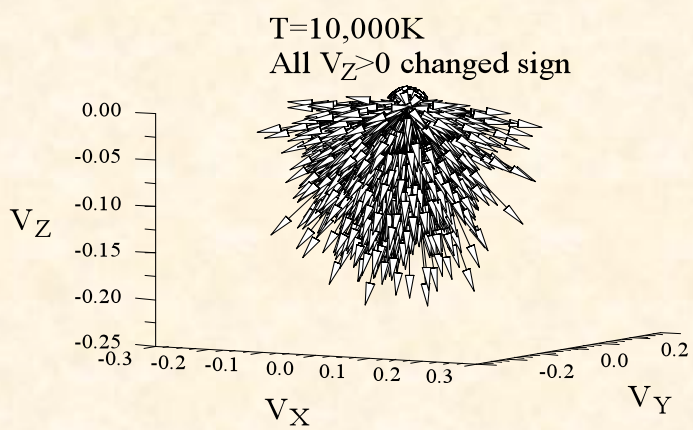


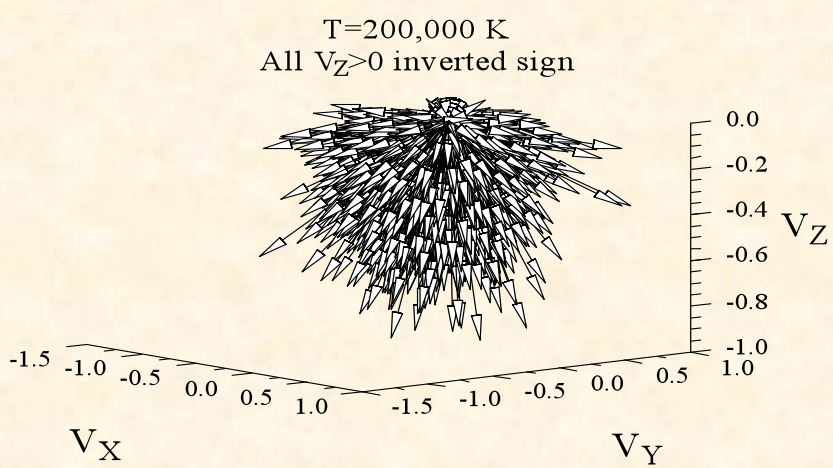
Ueda et al,2008

Impact plasma distributions (D atom): Examples









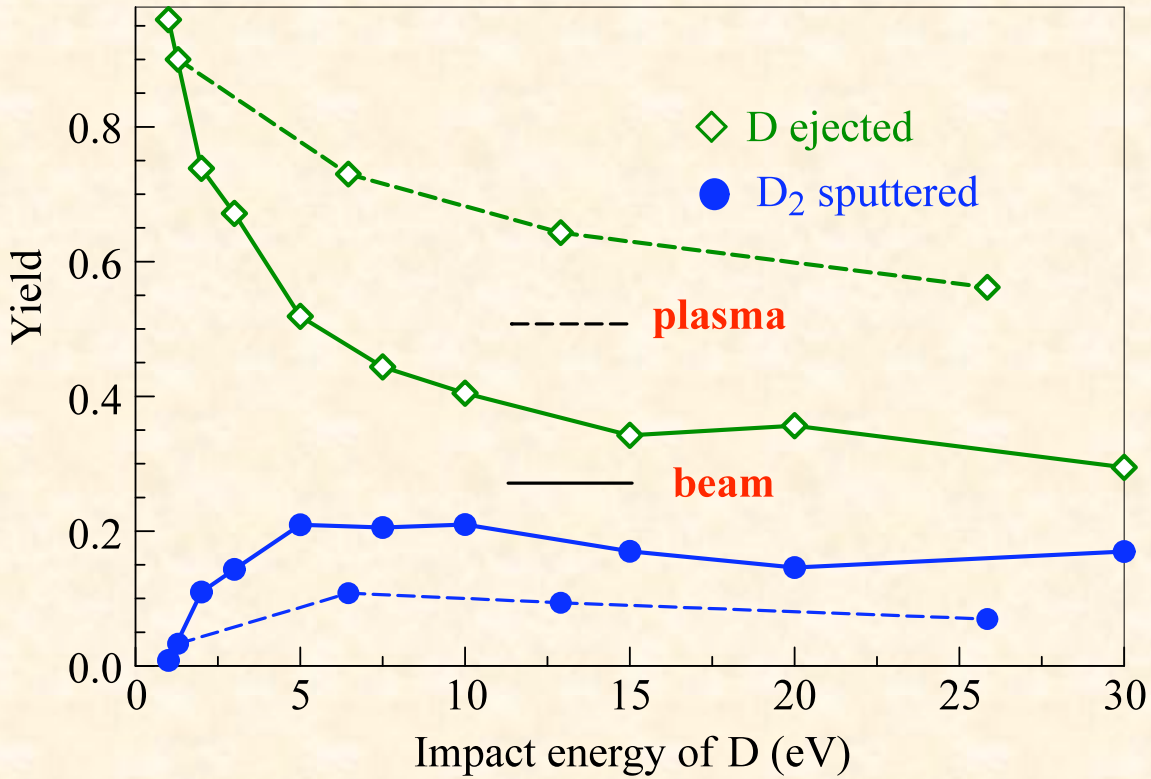
Plasma Irradiation!!!

Output (reflected) distributions of D

Distributions of sputtered hydrocarbons

Angular momentum distributions

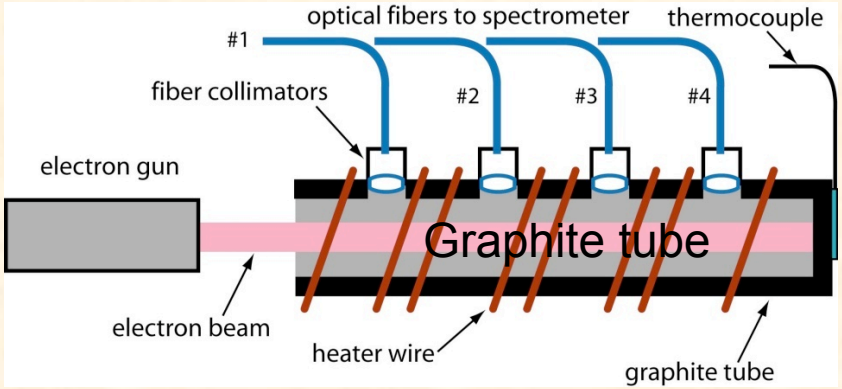
D2 sputtering and D re-emission with beam and plasma



With plasma irradiation:

Reflection significantly higher, sputtering smaller!!!

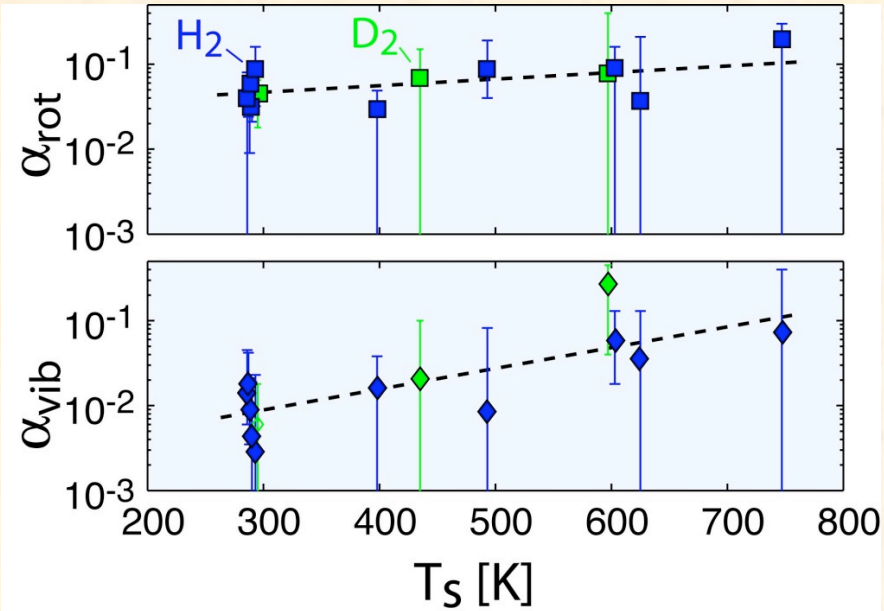
Plasma irradiation – 1st direct comp of atomistic calc with plasma experiment: designed by E. Hollmann (UCSD) 2008



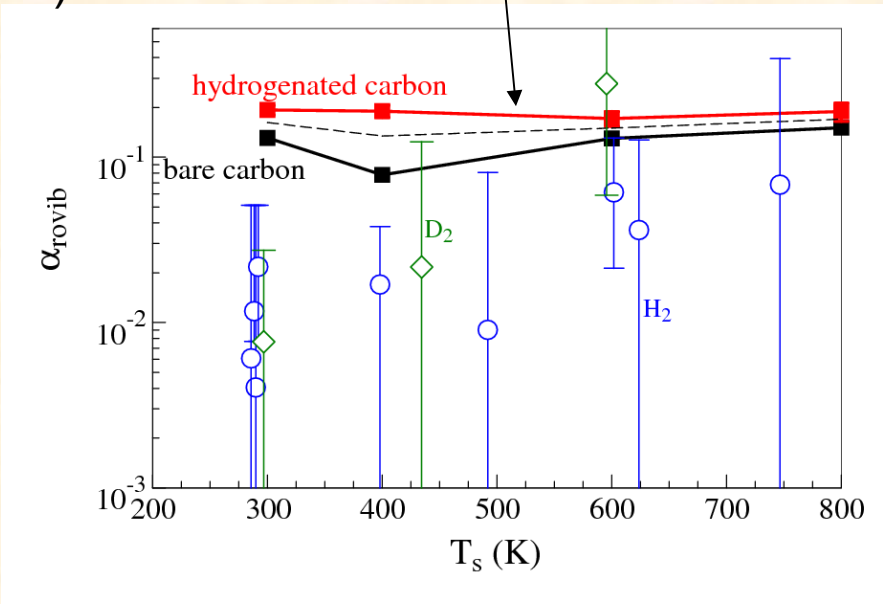
Accommodation coefficient

$$\alpha = \frac{T - T_0}{T_0 - T_s}$$

Measured (assumption Tv=5000K, Tr=Tk=800K)



MD simulated



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Modelling of high flux plasma-wall interaction is complicated by surface response to plasma bombardment

Incident plasma

- Multi-species, multi-state plasma
- Multi-component, multi-directional distribution function

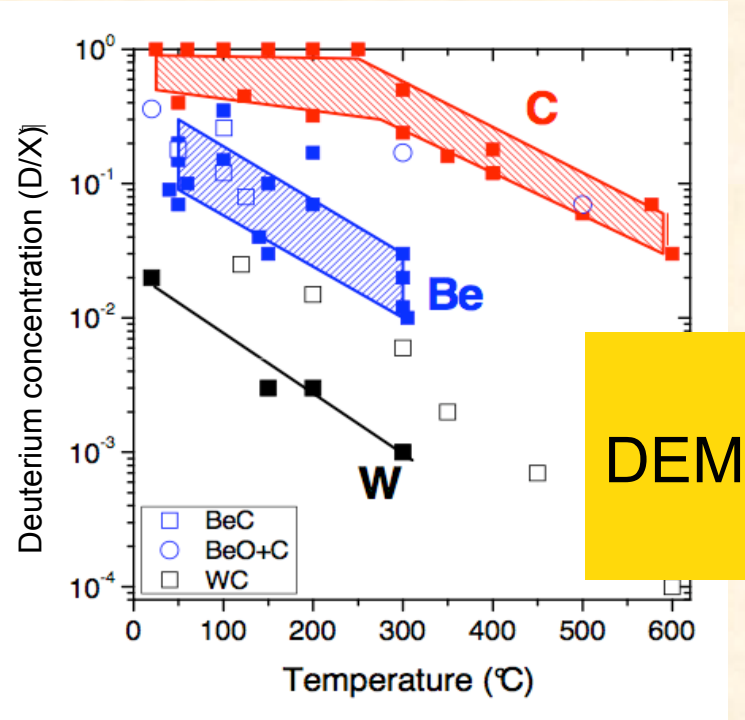
Evolving target

- History of irradiation, heating
- Surface deposition & damage

Products

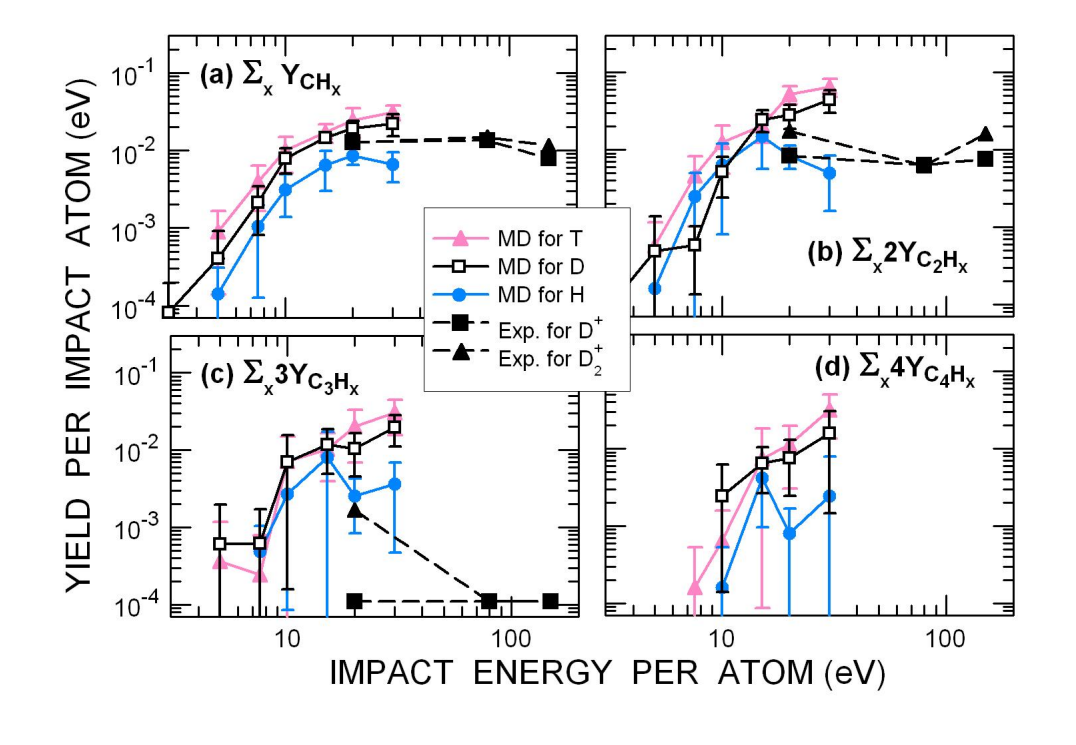
- Particle reflection, implantation, sputtering
- Synergetic surface chemistry

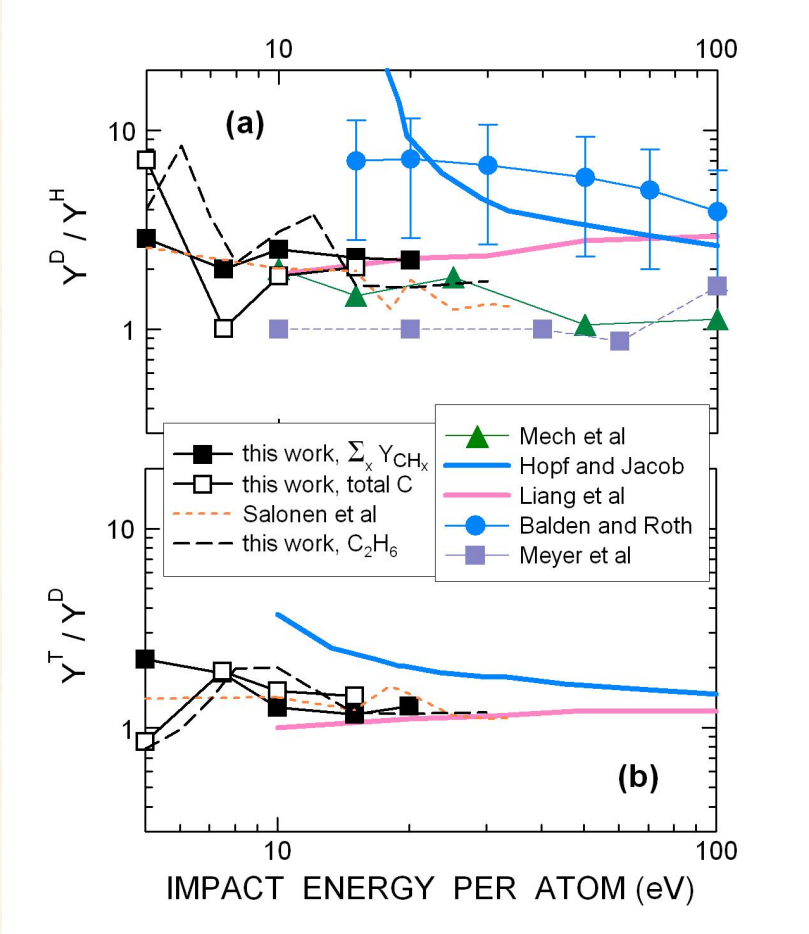
Reliability of extrapolation to DEMO depends on validation of theory with thorough experimental characterization



Retained deuterium concentration in C, Be and W co-depositio
n
conditions. (J. Roth et al., PPCF 50 (2008)103001)

ISOTOPIC EFFECTS





Smaller than expected!

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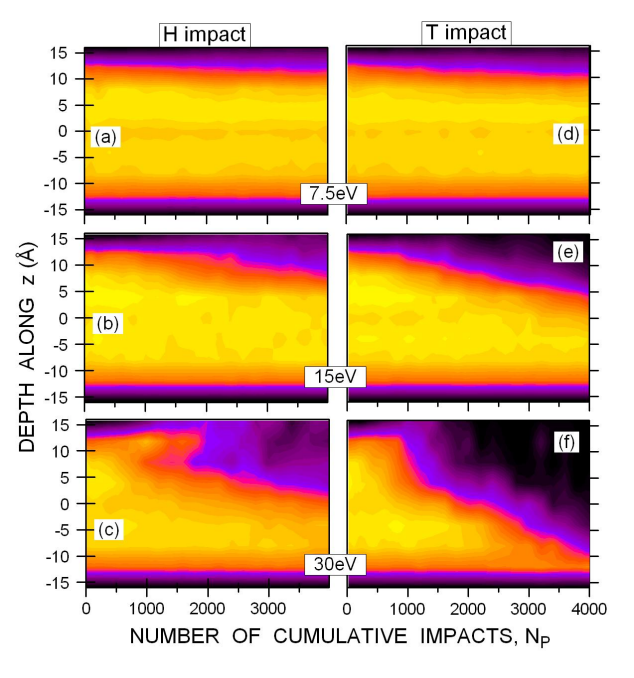
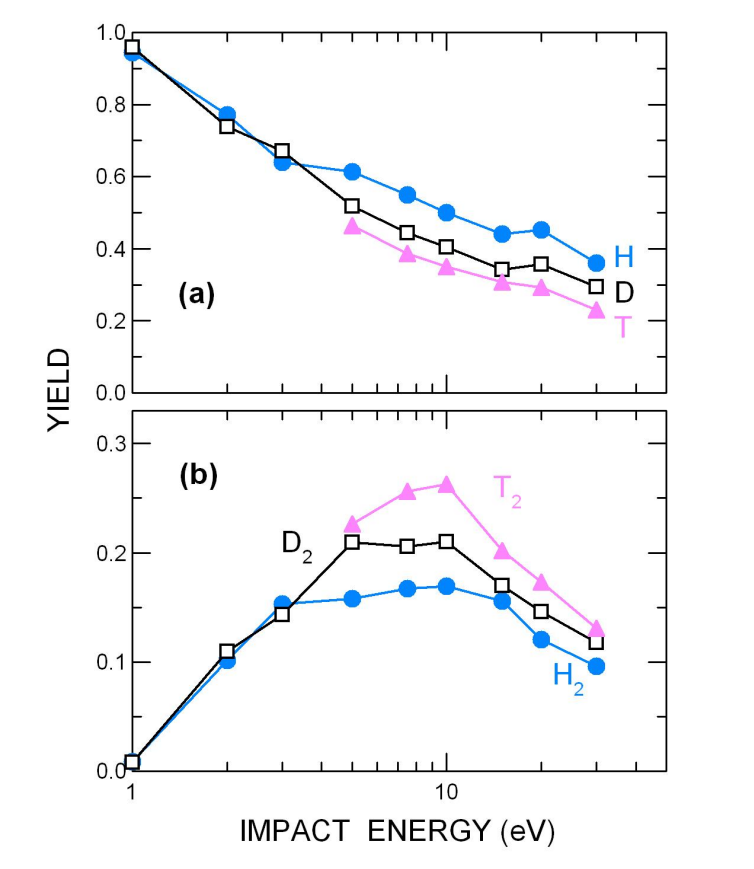
Consequently, "damages" by H and T impact comparable!



Emission of H and H2 by H impact



New materials, inclusion of quantum mechanical effects, long times, T…

Where do we see continuous challenges?

-New targets: C crystalline, polycrystalline structures; CFC, doped C, Tungsten, Beryllium …

target temperature variation

-New plasma particles: N (N^2), C, W, Be, inert gases

isotopic effects

-Development of new methods:

New potentials (C,W,Be,H) !!!!! (A. Allouche, K. Nordlund)

CNMS of ORNL ZBL corrections; Barrier corrections (done!)

Excited state MD

Charge transfer (impinging ions),

El. excitations of projectiles and target atoms

Expansion of computation capabilities

EXPERIMENTAL VALIDATION OF HIGH IMPORTANCE!!!

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Experiment

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F. W. Meyer, P. S. Krstic, L. I. Vergara, H. F. Krause, C. O. Reinhold, and S. J. Stuart Phys. Scr. **T128**, 50 (2007).
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L.I. Vergara, F.W. Meyer, and H.F. Krause, J. Nucl. Mater. **347** (2005) 118
L.I. Vergara, F.W. Meyer, H.F. Krause, P. Traskelin, K. Nordlund, and E. Salonen, J. Nucl. Mater. **357** (2006) 9.