PFC Sputtering Response Modeling for NSTX, C-MOD, DIII-D

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PURDUE UNIVERSITY

Collaborators

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LLNL: T. Rognlien

MIT: H. Barnard, B. Lipshultz, D. Whyte

ORNL: J. Canik, P. Krstic, R. Maingi

PPPL: H. Kugel, C. Skinner, D. Stotler, et al.

Why Model the US Tokamaks?

- Critically important to understand, predict, and validate sputter response of **high-Z** coated plasma facing components.

- In particular, ITER, DEMO likely highly dependent on tungsten sputtering response (and transient response). Need to validate predictions of high sputter redeposition fraction, low net erosion and low core plasma contamination.

- Good erosion/redeposition code/data agreement in numerous devices, e.g., for Be, C, W, in TFTR, JET, DIII-D; *but not with Mo in C-MOD* [J.N. Brooks, et al., PSI-19, J. Nuc. Mater (2010) t.b.p.] .

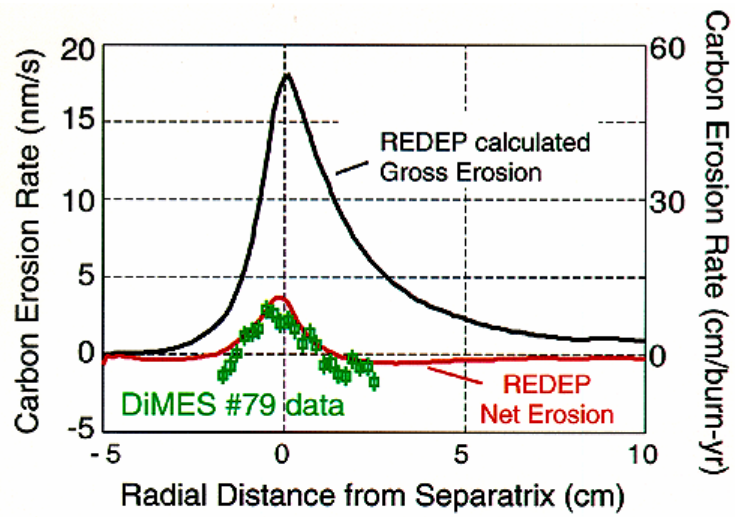
- **Liquid lithium** (& Sn, Ga) divertor surface is an important option for future fusion devices (Fusion Nuclear Science Facility, DEMO, etc.) –for high power and particle handling.

- The 3 major US tokamaks (supplemented by Lab devices). offer a major (but difficult) opportunity for model development and code/data validation.

DIII-D DiMES experiments modeling

DIII-D/DiMES probe is an important plasma/material interaction test facility.

DiMES probe



Exposure Conditions

Attached ELMing H-mode
0.7 MW/m²
$T_{e,OSP}$ = 70 eV

Sandia National Laboratories UCSD GENERAL ATOMICS

REDEP/WBC Code Matches the Features of Carbon Net Erosion at the DIII-D Divertor as Measured by DiMES
[J.N. Brooks, D.G. Whyte, Nuclear Fusion 39(1999)525]

NSTX Modeling

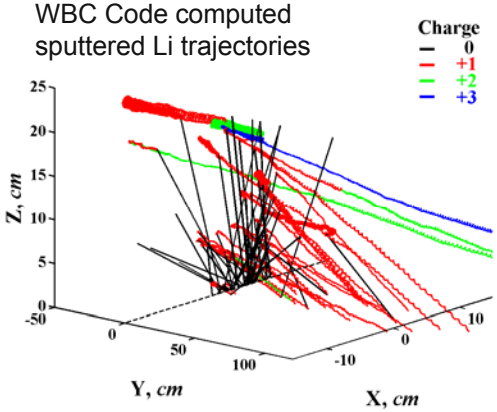
- Liquid Lithium Divertor (LLD) plasma/surface interaction analysis

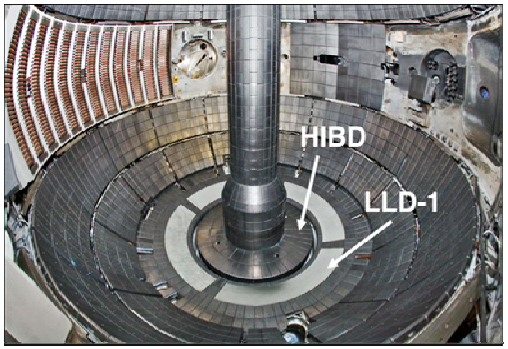
[J.N. Brooks, J.P. Allain, T.D. Rognlien, R. Maingi., J. Nuc. Mat. 337-339(2005)1053]

[J.P. Allain, J.N. Brooks, Nuclear Fusion 51(2011)023002]

  - *static liquid lithium response, low-D recycle plasma*

WBC Code computed sputtered Li trajectories





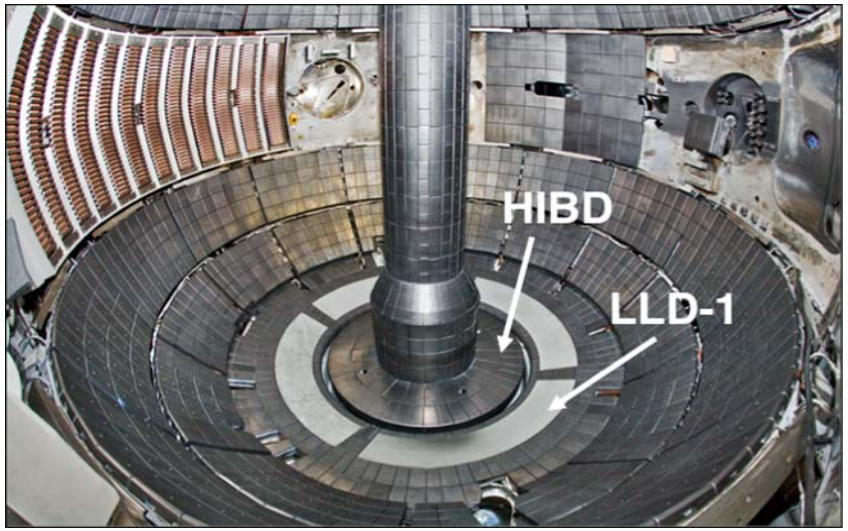
- **Lithium Inner Divertor (HIBD)**
  - *static (pure) liquid Li or solid Li surface, high D-recycle plasma (SOLPS/B2-IRENE, J. Canik ORNL)*

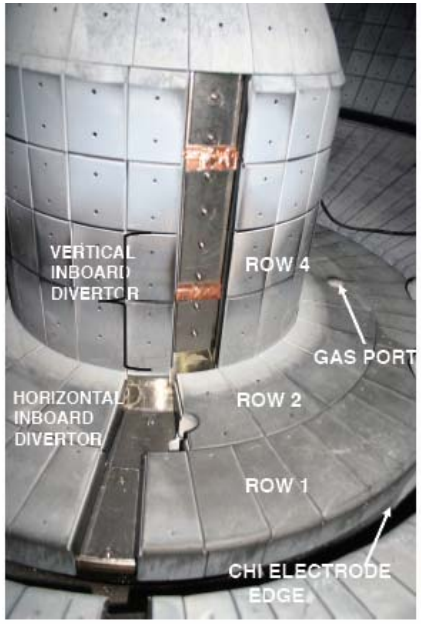
[J.N. Brooks, A. Hassanein, T. Sizyuk, J.P. Allain, 2nd Inter. Symposium on Li applications for Fusion Devices, PPPL, 4/11, Fus. Tech. submitted]

- **Molybdenum Inner Divertor and mixed material analysis**:
  - Li + C on Mo inner divertor, high-D-recycle plasma surface evolution: composition and sputtering

(ibid. and continuing)

REDEP/WBC NSTX Inner Divertor Analysis; with high-recycle plasma





- NSTX Horizontal Inboard Divertor (HIBD) carbon tiles replaced with molybdenum —To reduce carbon sputtering & core plasma carbon content.

- We are analyzing Mo, C, Li HIBD ("inner divertor") sputtering erosion and plasma contamination, with high-recycle plasma.

Concerns for NSTX analysis: *Much more difficult to model than future devices*

--- Transient conditions: ~1 second pulse

--- Small device–edge/boundary effects dominate

--- Lithium is not a flowing liquid (i.e., is static liquid or solid)

--- Many materials present (C, Mo, etc.)

--- Non-standard boundary conditions

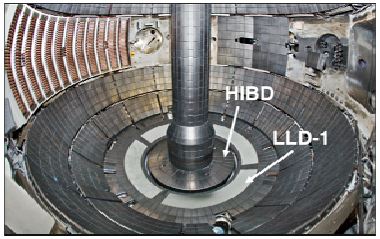
Lithium modeling issues

Lithium is the 2nd most complex surface material we have modeled (carbon is first due to chemical sputtering):

- D trapping/pumping—highly dependent on surface content/structure
- High vapor pressure
- Temperature dependent sputtering & evaporation
- Material-mixing issues: e.g. Li intercalation in carbon
- Liquid vs. solid issues
- Most (~2/3) sputtering is Li^+ ions
- Li^+ ion redeposition in sheath and re-emission at surface

REDEP/WBC Code Package analysis of three surface materials

NSTX inner divertor (HIBD), high-recycle regime



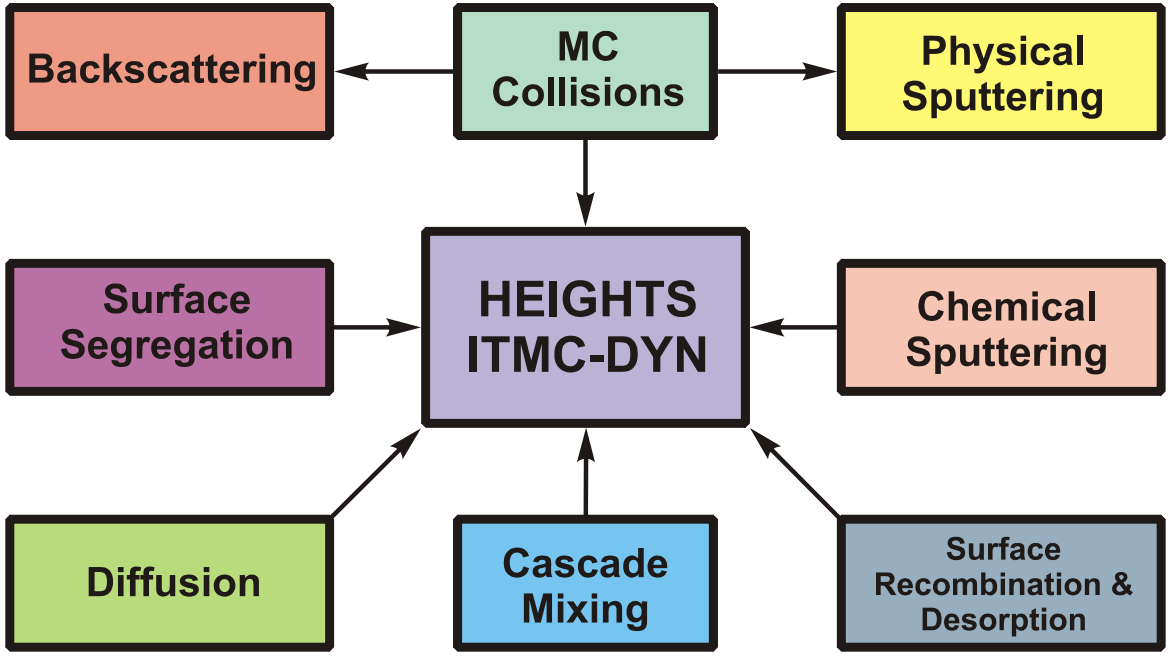
Parameter	Carbon	Molybdenum	Lithium
Ionization mean free path[a], mm	5.3	0.72	0.77
Gross erosion rate, typical, nm/s	20	15	200
Net erosion rate, typical, nm/s	2	0.5	5
Core plasma contamination potential[b]	$< 2 \times 10^{-3}$	$< 5 \times 10^{-5}$	$< 1 \times 10^{-3}$

[a] with 1% C^{+3} and 1% Li^{+2} plasma impingement
[b] normal-to-surface; for sputtered atoms ionized in divertor region.
[c] numerical bound

- C and Li net sputter erosion is about 5-10 times higher than Mo
- No material highly contaminates core plasma

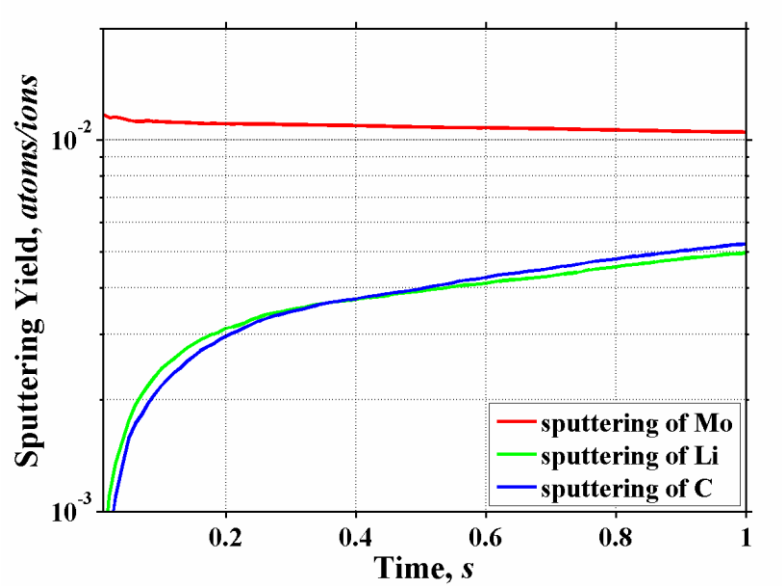
Dynamic evolution of mixed materials bombarded with multiple ion beams: ITMC-DYN Computer Simulation Package

ITMC-DYN Integrated Models

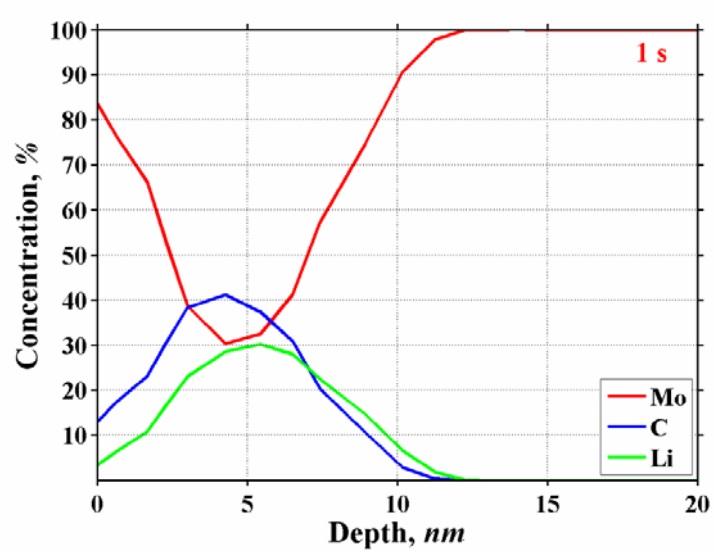


- A. Hassanein, "Surface effects on sputtered atoms and their angular and energy dependence", Fusion Technology 8 (1985) 1735.
- T. Sizyuk and A. Hassanein, "Dynamic analysis and evolution of mixed materials bombarded with multiple ions beams", J. Nucl. Materials, 40(2010)60
- T. Sizyuk and A. Hassanein "Dynamic analysis of mixed ion beams/materials effects on the performance of ITER-like devices", to be published J. Nucl. Mat. (2010)

ITMC-DYN analysis: Time dependent sputtering of NSTX Mo inner divertor (at strike point); with D, 1% C, 1% Li impingement



Time dependent sputtering

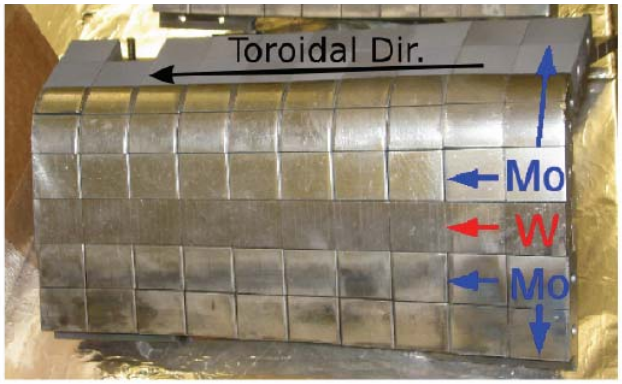


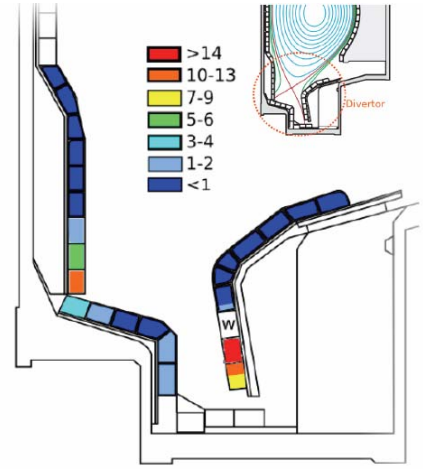
Spatial distribution of the deposited C and Li impurities in Mo substrate; at 1 second.

- Substantial carbon and lithium sputtering occurs by end-of-shot
- C and Li surface contamination extend to ~10 nm, by end of shot
- C and Li concentrations peak at ~ 5 nm depth and about equal the Mo concentration

W Migration in Alcator C-Mod

H. Barnard , B. Lipschultz, D. Whyte, MIT
(ITPA Seoul Korea, 2010)





Tungsten deposition, 10^{20} atoms / m^2

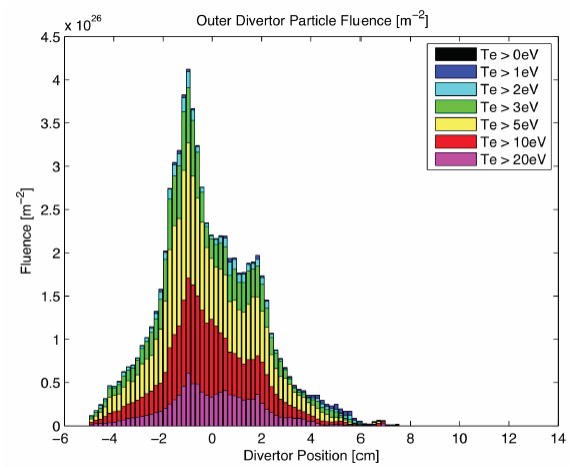
Toroidally symmetric tungsten tiles at/near outer divertor strike point. Exposed for ~10^3 s at various plasma conditions.

D +1% B plasma. Total ion fluence ~ 10^{26} D/m^2.

Post-exposure deposition measured by external MeV ion beam. (2 MeV protons; PIXE, PIGE)

A net effective thickness 4×10^{21} W/m^2 $\approx$ 60 nm was removed.

Modeling goal: Compare code/data erosion and impurity transport. Key focus on net/gross erosion



Plasma shot Te histogram

Modeling of C-MOD Tungsten Migration

- Initial steps:
  1) BPHI code analysis of C-MOD outer divertor sheath conditions and boron ion impingement.
  2) ITMC code computation of B on W sputter yields and velocity distribution functions. (Pure W assumed)
  3) Tungsten gross erosion, rough estimate; per fluence data and above results.

- Next: Detailed REDEP/WBC code package analysis of C-MOD tungsten sputtering, transport, gross and net erosion.

  ---including-self-consistent self-sputtering, B/W & Mo/W deposition/erosion, radial electric field, other effects.

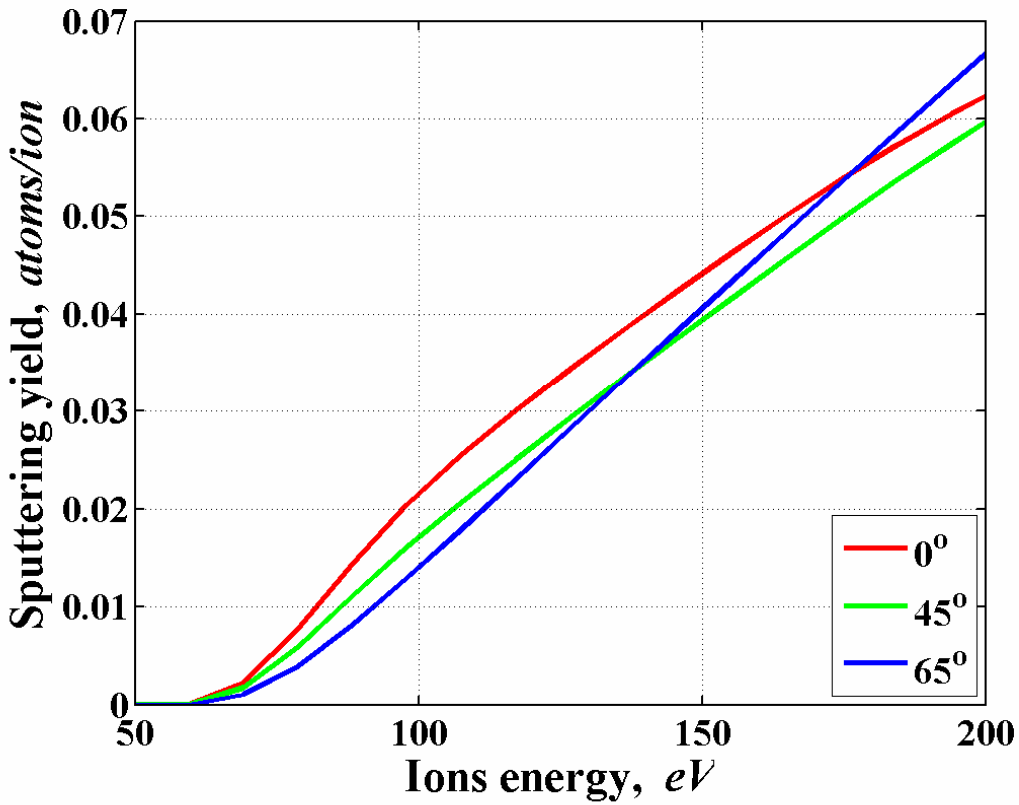
  ---compute tungsten transport to outer and inner divertor; compare with data.

C-MOD Tungsten Migration Analysis--Initial results

- BPHI code* analysis of C-MOD sheath at outer divertor, with strong, highly oblique, magnetic field. B ~ 6 T @ 1º (from tangential), Te = 5-20 eV conditions.
  - Result: dual sheath structure obtains (magnetic + Debye regions); sheath potential $e\Phi \sim 3kT_e$
  - B^{+3} ions, (thermalized boundary conditions at sheath start) accelerated through sheath: average impingement angle ~65° (from normal), av. energy ~150 eV for T_e=10 eV

* J.N. Brooks, D. Naujoks, Physics Plasmas 7(2000)2565

ITMC code computation (Sizyuk, Hassanein) of B on W sputtering
(KrC potential + LSS for electronic stopping)



- C-MOD-relevant sputter yields of order 0.05 W-atoms/B-ion

C-MOD Tungsten Migration Analysis-- Initial gross erosion estimate

- Gross erosion rough estimate:

  B^{+3} fluence ~10^{24} B/m^2 (for 1% B/D) (Barnard, Whyte, et al.)

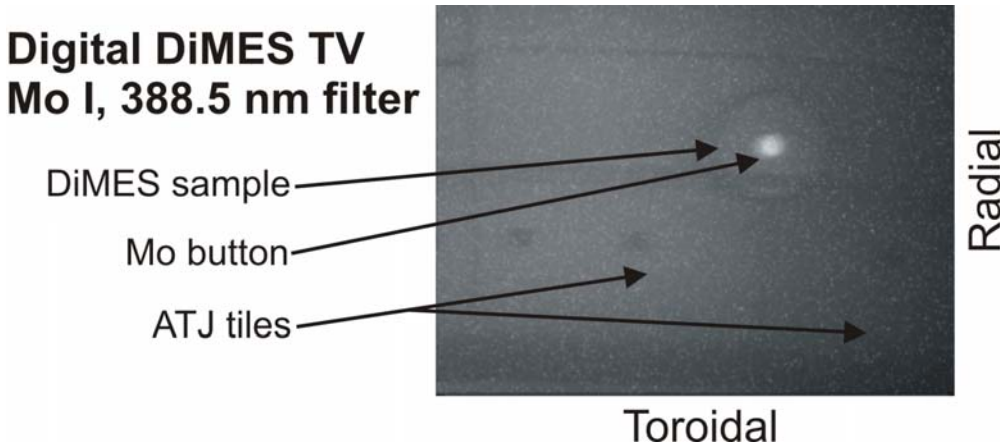
  Y~ 0.05 W/B, sputter yield

  $\Rightarrow$ ~5×10^{22} W/m^2 sputtered W fluence $\Rightarrow$ **~800 nm gross erosion**

  – **factor of ~10 reduction from data-inferred ~60 nm net erosion**

  – **Thus, consistent with >90% redeposition fraction. Encouraging.**

DIII-D DiMES high-Z (Molybdenum) erosion experiment



- Conducted August 1, 2011; GA, SNL
- Purpose: test if net erosion << gross erosion for high-Z material.
- 1 cm dia, 25 nm deposited Mo metallic film on Si substrate, on DiMES probe.
- 7 Mo exposure shots, 4 s/shot, well-characterized, same plasma conditions.
- Real time, Mo-I line emission spectroscopy assessment of gross sputter erosion (GA); post test, ex-situ probe measurement of net erosion (Wampler et al, SNL.)

- Simulation started, J. Brooks et al. (Purdue) with GA et al. collaboration. Then, code/data comparisons.

Conclusions- *PFC Sputtering Response Modeling for NSTX, C-MOD, DIII-D*

- **NSTX: Li, Mo, C divertor surfaces under analysis.**

  --- Lithium surface—solid or liquid, for low or high D recycle plasma—has high erosion but low core plasma contamination potential (~0.1-1%).

  --- A molybdenum surface may be substantially changed, in 1 second, by C and Li impingement. Mo core plasma contamination by sputtering appears low (<0.01%), in any event. (Not clear if Mo substantially reduces NSTX core plasma carbon content).

- **C-MOD Tungsten tile experiment being analyzed. Initial result encouraging-code/data both indicate high redeposition fraction. Detailed analysis underway.**

- **DIII-D/DiMES-important Mo gross/net sputter erosion experiment performed-detailed simulation underway.**

- **All devices—key research thrusts include improved diagnostics, material mixing models/codes, supercomputing.**