

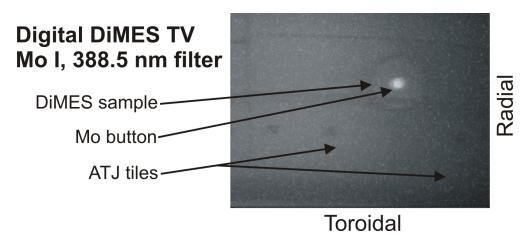
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DIII-D DiMES high-Z (Molybdenum) erosion experiments



- 3 experiments conducted (GA, SNL): focus here on the August 1, 2011 experiment
- Purpose: test if net erosion << gross erosion for high-Z material.</p>
- 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.
- Post exposure, ex-situ probe measurement of net erosion (Wampler et al, SNL.)

[1] J.N. Brooks, A. Hassanein, T. Sizyuk, "Advanced simulation of mixed-material erosion/evolution and application to low and high-Z containing plasma facing components", PSI-20, J. Nuc. Mat. to be published.

[2] P.C. Stangeby et al., "An experimental comparison of gross and net erosion of Mo in the DIII-D divertor", ibid.

[3] W. R. Wampler et al., "Measurements of net erosion and redeposition of molybdenum in DIII-D", ibid.

[4]. D.L. Rudakov et al., "Reduction of Net Erosion of High-Z Divertor Surface by Local Redeposition in DIII-D", IAEA2012, to be presented.





TABLE I. Features of the 3 Mo experiments.

date	exposure time [s]	initial thickness of 1 cm sample [nm]	probe data. T _e -max [eV], n _e -max [10 ¹⁹ m ⁻³]	Mol filter passband [nm]	with 1 mm sample
8/1/2011	28	24.16	30, 1.5	10	no
4/23/2012	12	23.81	no data	1	no
5/1/2012	4	16.13	40, 1.2	1	yes



DiMES probe for 5/1/12; 1 cm and 1 mm Mo spots on carbon probe





Mixed-material response is key to understanding DIII-D Mo results

- We analyzed D/Mo/C divertor plasma interactions with mixed-material surfaces using advanced modeling of time-dependent surface evolution and erosion*.
- Simulations use the REDEP/WBC sputtering erosion/redeposition code package coupled to the HEIGHTS package ITMC-DYN mixed-material formation/response code, with plasma parameter input from codes and data.
- The DIII-D/DiMES probe experiment simulation predicts that sputtered molybdenum from a 1 cm dia. central spot quickly (~ 4 sec.) saturates in the 5 cm dia. surrounding carbon probe surface, with subsequent resputtering and transport to off-probe regions, and with high (~50%) redeposition on the Mo spot.

Predicted Mo content in the carbon agrees well with post exposure probe data.

*Mixed-material work partially supported by the U.S. Department of Energy Office of Fusion Energy Sciences, and by Purdue University.





DIII-D Mo-DiMES: Key Data to be explained

1. Net erosion rate, Mo sample: 0.4 nm/s

2. Gross/Net erosion rate: ~2.0

- 3. Fraction of net eroded Mo found in DiMES "probe cap" (carbon portion of probe): 19% (Thus, 81% not on probe).
- 4. Mo deposition profiles on DiMES graphite surface.





Simulation Method

REDEP/WBC code package, full-kinetic (3D/3V), impurity sputtering, transport, sheath structure, etc, with ITMC-DYN input/output

ITMC-DYN: HEIGHTS-Package BCA code accounting for time-dependent changes in target composition, due to penetration and mixing, scattering, reflection, sputtering, thermal diffusion, hydrogen isotope molecular recombination, and surface segregation.

DIII-D/DiMES experiment of Aug. 1, 2011

1 cm diameter Mo spot on 5 cm dia. graphite probe

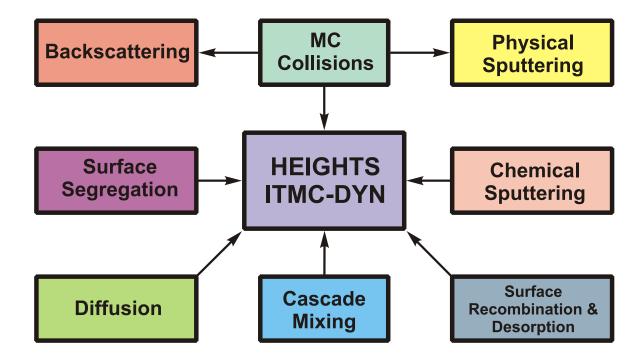
Background plasma from codes/data: 7 shots x 4 seconds/shot = 28 s exposure; Te=30 eV, Ne=1.5 x10¹⁹ m⁻³ 1% C⁺³/D⁺, magnetic + Debye sheath, Mach-1 flow Other REDEP/WBC etc. plasma parameters





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)





Coupled simulation: WBC/ITMC

- Mo atoms launched randomly from the 1 cm dia. spot, per ITMC-DYN energy and angle probability distributions for C^{+3} on Mo sputtering
- Mo ionization and transport then followed.
- Ion history terminates if redeposited on the Mo spot or deposited off-probe.
- Mo ion incident on the probe carbon is re-sputtered per ITMC-DYN calculation, which also takes into account the simultaneous D ion flux.
- 10^6 histories/run, with spot-sputtered particle numerical weighting calibrated to the measured net erosion rate of 0.4 nm/s.

Key simulation outputs are redeposition rates, gross/net erosion ratio, deposition profles, and Mo content in the carbon.





DiMES WBC/ITMC Coupled Modeling-cont.

Moderate computational resources and numerical requirements needed/used here--due to small divertor area involved, near-constant plasma parameters, limited exposure time.

[Most future, mixed-material simulations would need petascale computing]





Table 1 REDEP/ITMC analysis summary for DiMES probe sputtered molybdenum, 10 $^{\rm 6}$ histories

Parameter	Value	
Ionization mean-free-patha	1.2 mm	
Charge state⋼	1.7 (0.73)	
Energy ^b	156 (86) eV	
Incidence elevation angle (from normal) ^b	22 (11)	
Transit time∘	0.98µs	
Redeposition fraction on Mo spot	0.54	
Redeposition fraction on divertor	~1	
Mo content in carbon portion of probe; at end of discharge	0.75 x10 ¹⁶ atoms	

^a For sputtered Mo atoms, perp. to surface, from Mo spot and carbon

Average (and standard deviation where indicated) for redeposited Mo ion

Average for Mo ions, ionization-to-redeposition

Including probe; essentially 100% redeposition on divertor

---- High redeposition fraction on 1 cm dia. Mo spot

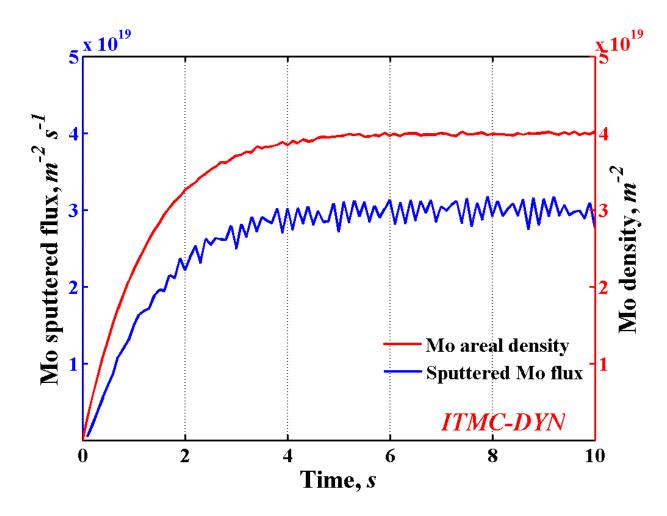
---- ~ 2-to-1 gross/net erosion ratio predicted

--- Essentially zero core plasma contamination predicted





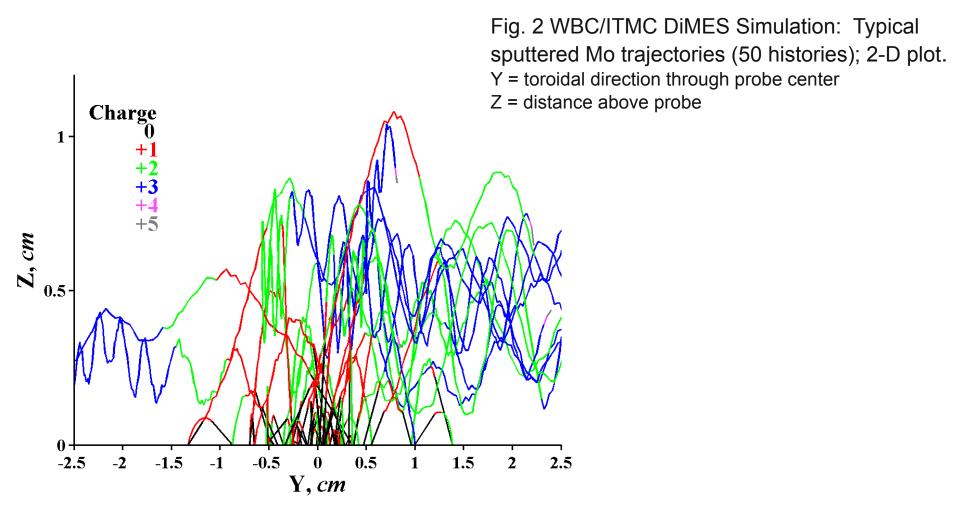
Fig. 1 Time-dependent sputtered Mo flux from, and areal density in, DIII-DiMES carbon probe surface, for $3x10^{19}m^{-2}s^{-1}$ incident Mo ion flux. WBC/ITMC simulation (at typical point near Mo spot).



•Steady-state reached in ~ 4 seconds







Trajectories show:

- Approximately straight line motion from sputtering to first ionization.
- Ion gyro-rotation, charge-changing, and velocity-changing collisions with the background plasma.
- Resulting spot-redeposition, on-probe non-spot redeposition and re-sputtering, and offprobe transport.





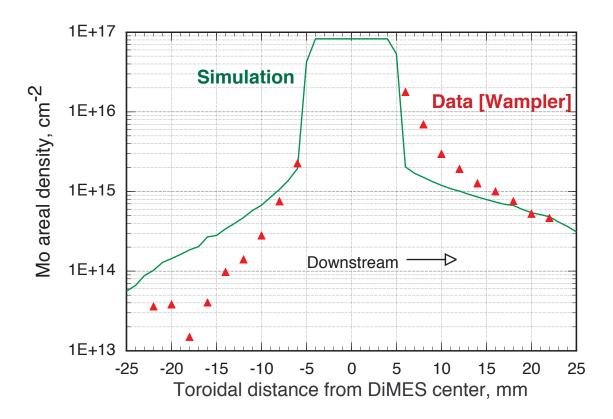


Fig 3 DiMES Mo areal density at end of 28 s exposure; along toroidal direction

---Good code/data match to Mo content in the carbon; 0.75×10^{16} vs. 1.1×10^{16} Mo atoms.

---"OK" code/data agreement to Mo toroidal profile-higher predicted upstream deposition.

PURDUE



W Migration in Alcator C-Mod



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

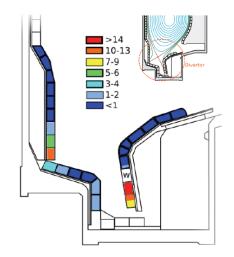
D +1% B plasma. Total ion fluence ~ 10^{26} D/m^{2.}

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

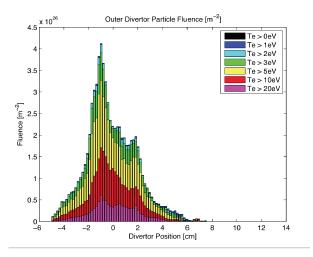
A net effective thickness $4x10^{21}$ W/m² ≈ 60 nm was removed.

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

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



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



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.
 - Initial results, consistent with >90% redeposition fraction. Encouraging.
- Underway: Detailed REDEP/WBC code package analysis of C-MOD tungsten sputtering, transport, gross and net erosion.

---including-self-consistent self-sputtering, convolution over discrete plasma conditions.

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





ITER-PFC Modeling Issues

- A key PFC issue is the effect of the ~700 m² wall-sputtered beryllium on the ~50 m² tungsten outer divertor, this potentially affecting Be/W alloy formation, thermal properties, divertor erosion, and T/Be codeposition in re-sputtered and off-divertor deposited beryllium.
- A previous study—using a simplified material response model—indicated no significant Be growth over most of the outer tungsten divertor, but with high Be growth at the strike point [J.N. Brooks, J.P. Allain, J. Nuclear Materials, 390-391 (2009)123]. *Generally encouraging results, but uncertain.*
- High-confidence, predictive ITER analysis can be performed with the advanced simulation method used here, however, the numerical issues become orders of magnitude greater. This is due to the ~50 cm long ITER divertor, with highly varying plasma parameters—compared to the 5 cm DiMES probe with near constant parameters. (An added complication for ITER is the multiple particle impingement, due to D, T, He, and any trace impurity.)
- An ITER full mixed-material divertor evolution study would require petascale computation.





Conclusions

- It is clear that mixed-material formation and plasma/surface interaction are key issues for fusion.
- We modeled this with advanced simulations using coupled erosion/redeposition and surface response code packages; but still with numerical simplifications-adequate for the small-area DiMES geometry.
- For DIII-DiMES, the analysis explains the important scientific result of high-Z material high-redeposition, quick saturation of W in probe C, and resulting transport of Mo to off-probe divertor surfaces.
- Results appear encouraging for high-Z material (W) use in ITER: low net sputter erosion, very low core plasma contamination.
- Predictive analysis for other mixed-material situations, such as ITER Be/W, and NSTX Li/C/Mo, with large area plasma facing surfaces, is highly amenable to our advanced simulation technique, but would require petascale computing.



