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Global modeling of wall material migration following boronization in NSTX-U

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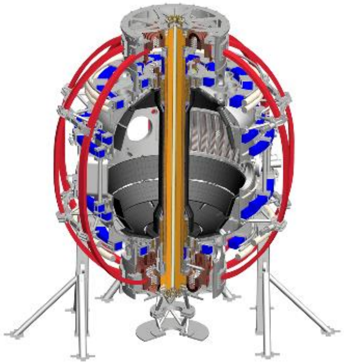
für Plasmaphysik



MOTIVATION

Plasma-wall interactions: a challenge for fusion that demands an integrated modeling approach

- Plasma-wall system is highly coupled, but operates on a wide range of length (10^{-10}-10^{2} m) and time (10^{-9}-10^{4} s) scales
- Integrated simulations must make use of one of two approaches:
  1. Exascale computing
  2. Reduced models ← This work
  - Caveat: Most reduced models have a large number of free parameters, which makes reaching ironclad conclusions difficult

- WallDYN is a global integrated mixed-material reduced model that has shown great promise in high-Z devices (JET-ILW, AUG, ITER)

  [K. Schmid JNM 2011], [K. Schmid NF 2015], [K. Schmid JNM 2015], [G. Meisl NF 2016]

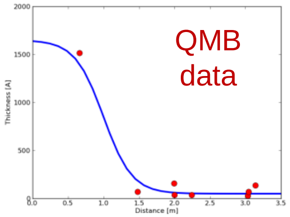
- Improvements have now been added to WallDYN that allow it to better capture the evolution of thin films used in wall conditioning
  - Wall conditioning and impurity control (especially oxygen) are persistent challenges for every device
  - Lower impurity influx means better plasma performance
  - Validated models can help optimize this process

BORONIZATION IN NSTX-U

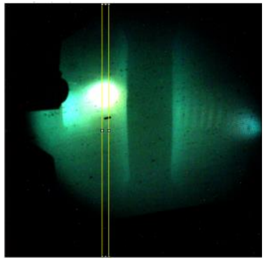
Boronization was used in NSTX-U to control impurity influx from the PFCs

- NSTX-U conditioned with deuterated trimethylboron (dTMB) injected into dual-anode He GDC; leads to thin film formation on walls
  - $B(CD_3)_3$: 17% boron by mass
  - MAPP XPS measurement post-boronizations: 60%C / 35%B / 5%O
  - “Full” boronization: 9.0g dTMB, ~weekly
  - “Mini” boronization: 1.8g dTMB, ~nightly
- Deposition highly peaked near GDC electrodes, but is more uniform when using multiple electrodes

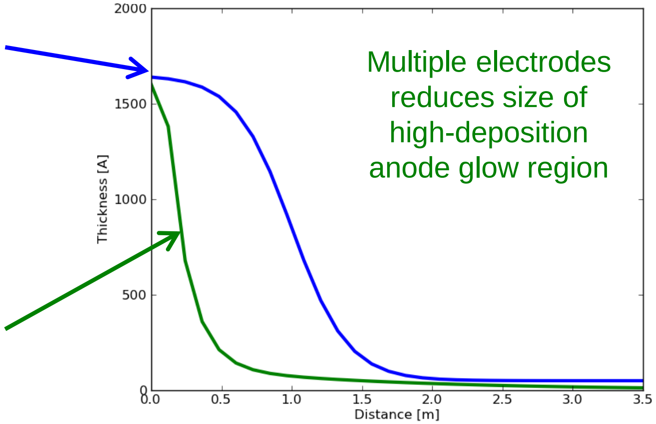
One anode



Two anodes

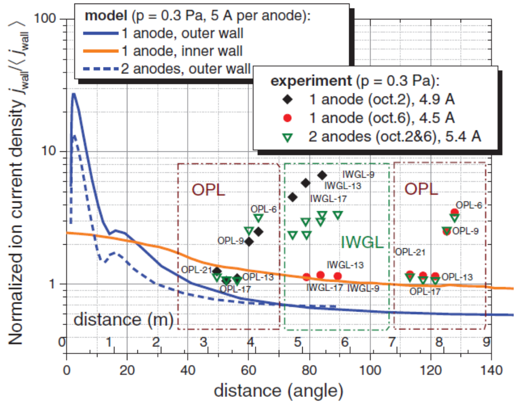


Per-anode deposition probability



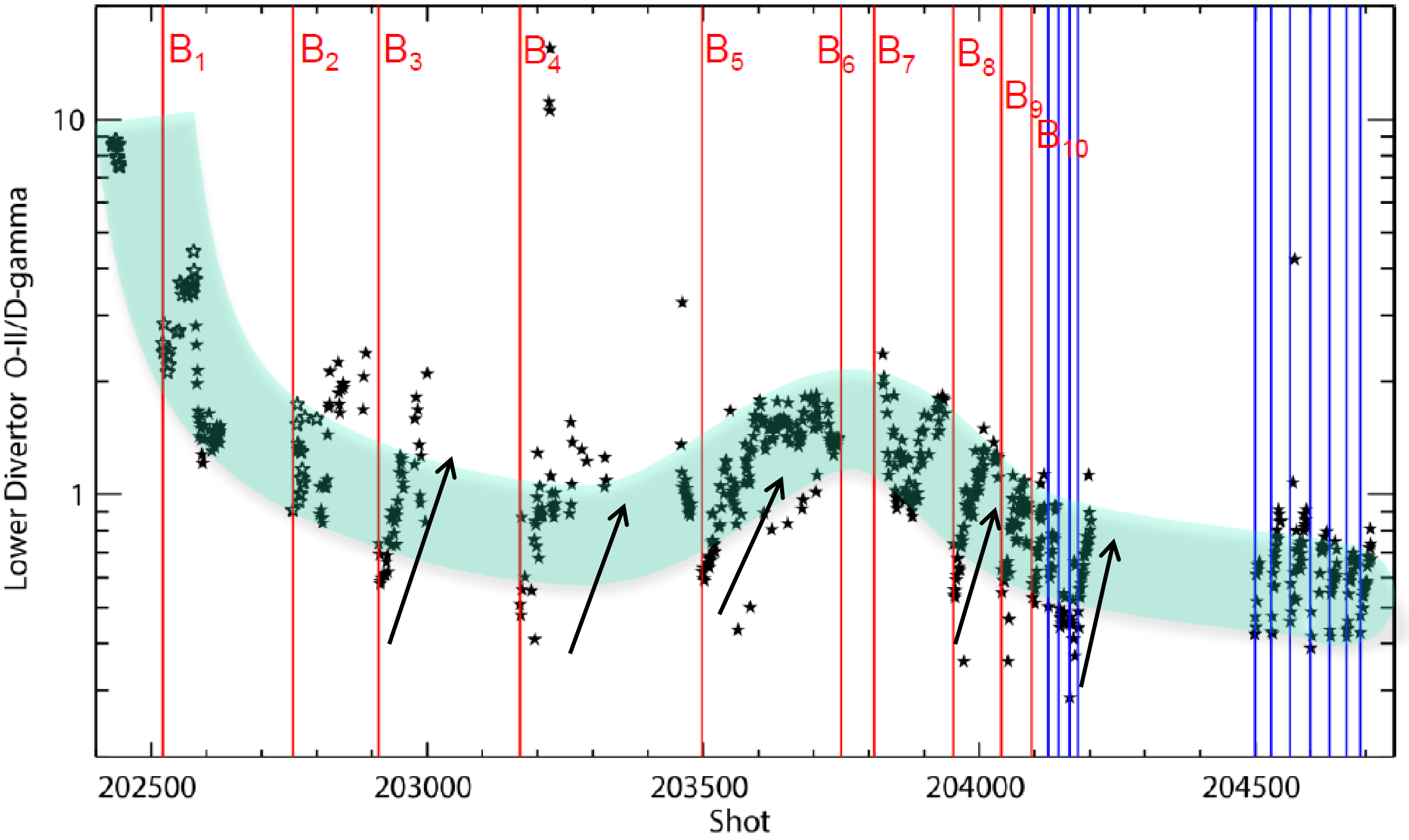
Multiple electrodes reduces size of high-deposition anode glow region

Comparable to 1 vs 2 anode JET results



[Kogut PPCF 2015]

Filterscope data from FY2016 campaign show increasing impurity influx between boronizations



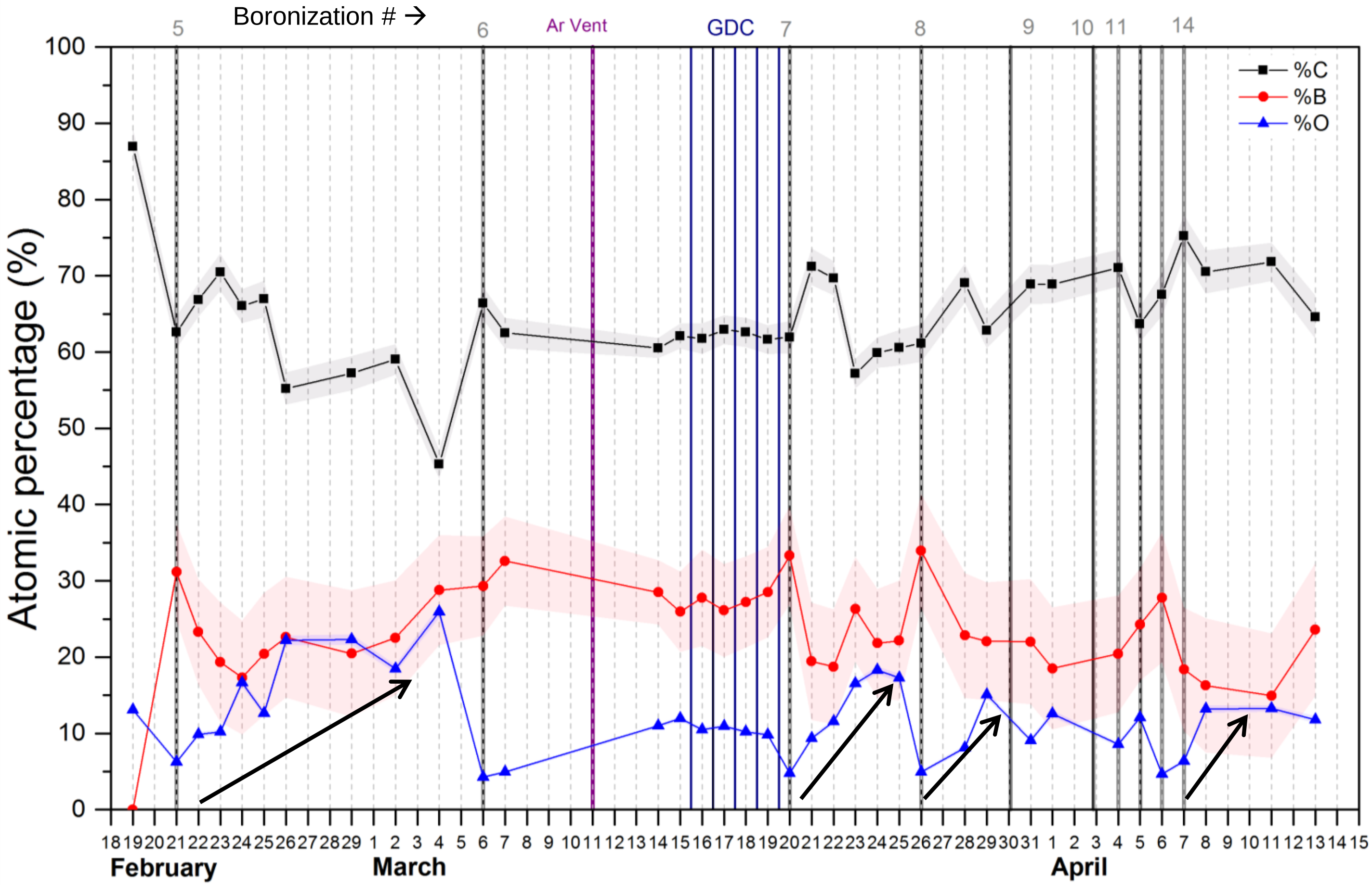
Full Boronization

Mini Boronization

Note: Langmuir probes inactive most of campaign → precludes absolute calibration of spectroscopic diagnostics

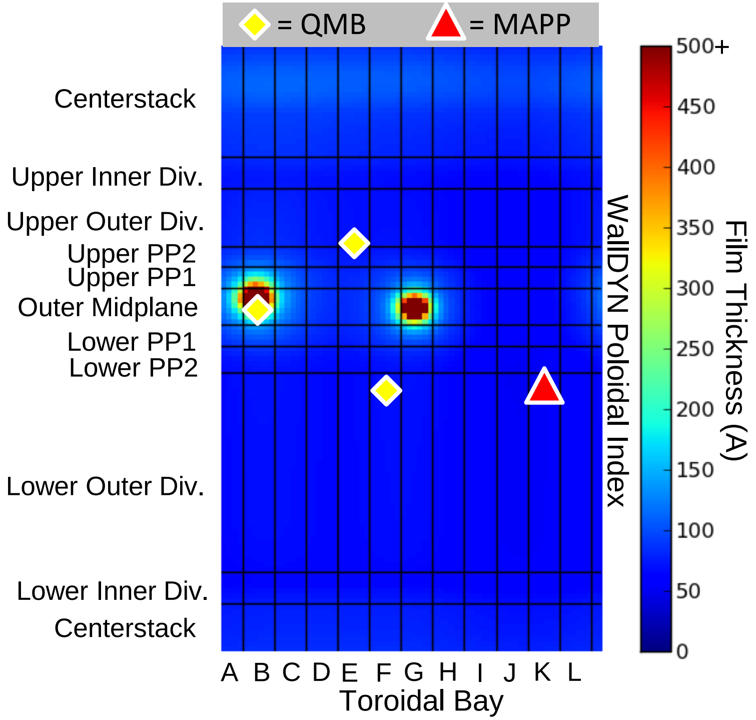
- Divertor filterscopes observed sharp decrease in OII/D-γ signal after boronization, with return to pre-boronized O levels after plasma exposure
  - Faster deconditioning following mini boronization than following full boronization

MAPP XPS data from FY2016 campaign corroborates filterscope trends



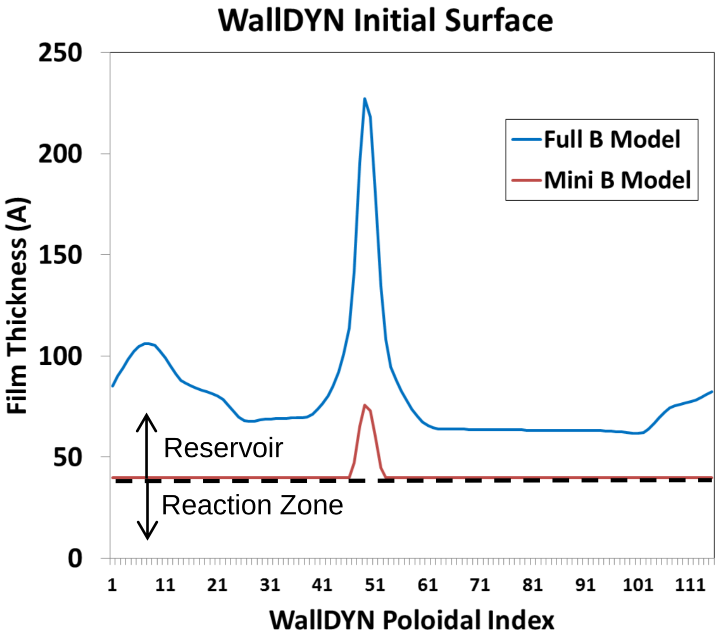
- MAPP XPS observed similar trends in total surface oxygen concentration on *in situ* lower divertor material probe
  - Note: XPS information depth ≈ Ion penetration depth ≈ WallDYN reaction zone width ≈ 4 nm

Boronization model developed that reproduces observed thin film deposition



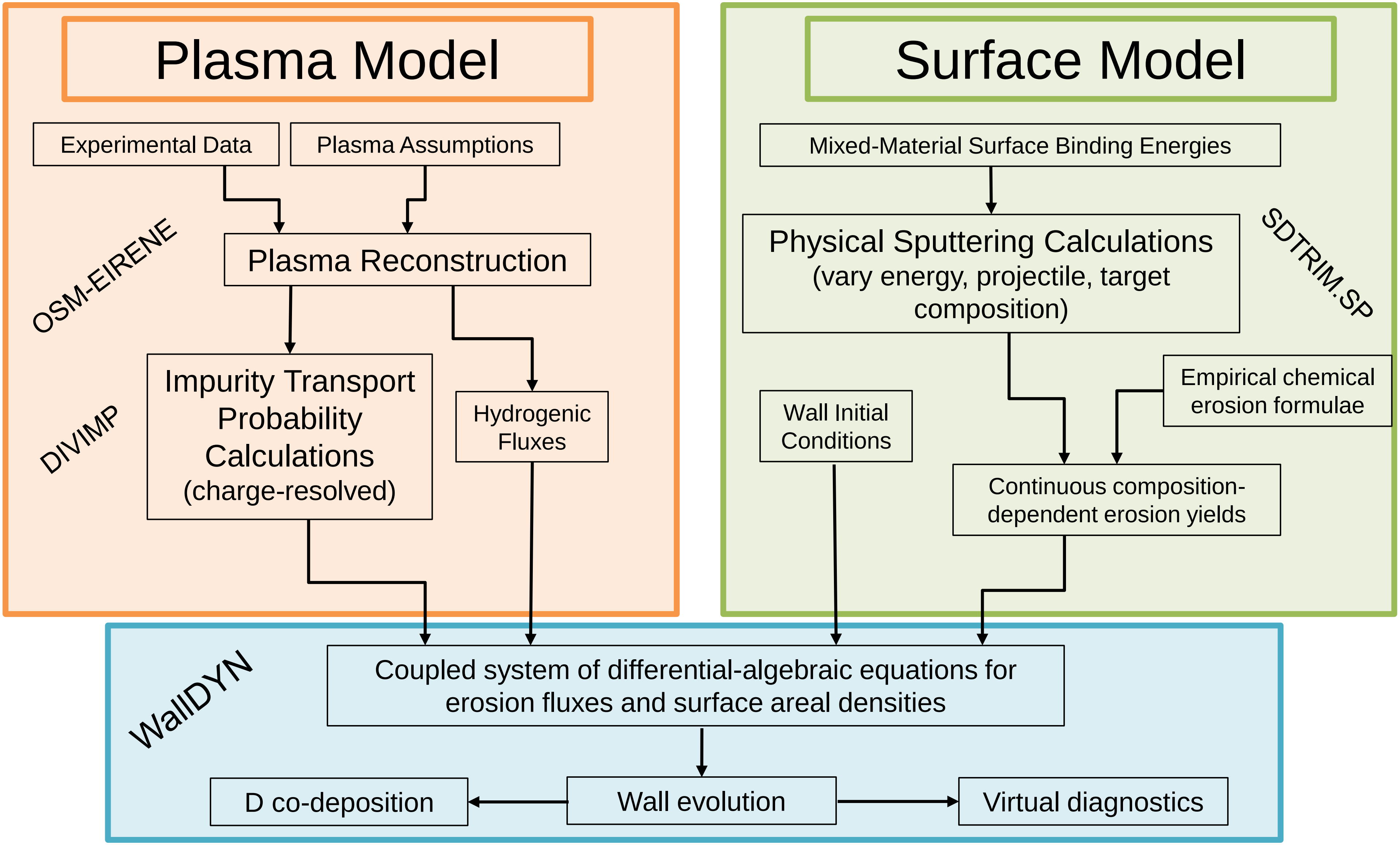
- Constrained by spatial distribution probability, film thickness scaled to match QMB data
  - Note: Only accounts for ~30% boron injected as dTMB
- Film composition: 60%C / 35%B / 5%O (from MAPP)
- Toroidally averaged for use in WallDYN

Full Boronization	B Mid	E Top	F Bot
Exp. QMB	1093 A	66 A	67 A
Model	1096 A	71 A	69 A
Mini Boronization	B Mid	E Top	F Bot
Exp. QMB	364 A	30 A	7 A
Model	365 A	40 A	40 A



WALLDYN MODEL

WallDYN: An integrated global model for mixed material migration



Plasma Model

Experimental Data

Plasma Assumptions

Plasma Reconstruction

OSM-EIRENE

Impurity Transport Probability Calculations (charge-resolved)

DIVIMP

Hydrogenic Fluxes

Surface Model

Mixed-Material Surface Binding Energies

Physical Sputtering Calculations (vary energy, projectile, target composition)

SDTRIM.SP

Empirical chemical erosion formulae

Wall Initial Conditions

Continuous composition-dependent erosion yields

WallDYN

Coupled system of differential-algebraic equations for erosion fluxes and surface areal densities

Wall evolution

D co-deposition

Virtual diagnostics

WallDYN parameterizes plasma impurity transport with DIVIMP 2D Monte Carlo code

- 20k neutrals launched from each wall bin
  - Energy and angular distribution typical of sputtered particles
  - Deposition location, charge state recorded
- R ≡ Fraction of eroded flux from “source” that ends up in a certain charge state at “destination”
- 1 Algebraic equation for influx of each element & charge state:

$$\Gamma^{IN}_{wall,elem}(t) = \sum_{source} R^{wall}_{source} * \Gamma^{OUT}_{source,elem}(t)$$

- Assumptions:
  - Impurity concentrations are low enough not to disturb plasma (“trace impurity limit”)
  - Plasma transport timescale << wall evolution timescale
  - Plasma does not change in time

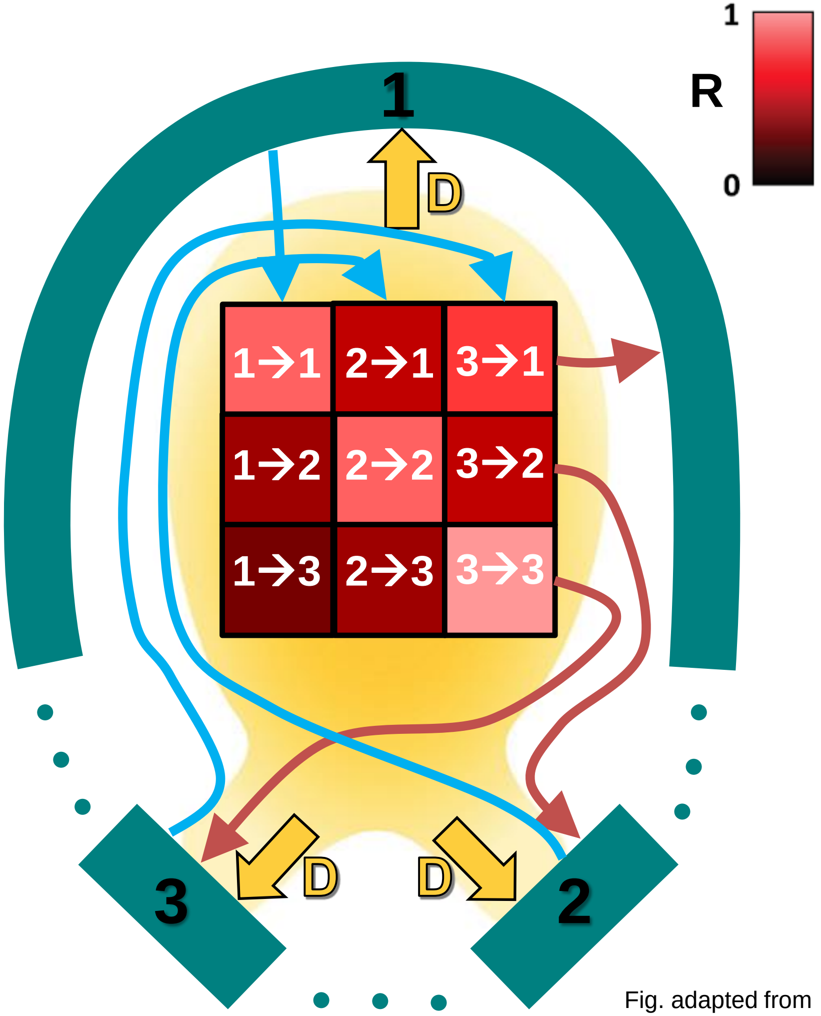


Fig. adapted from Meisl NF 2016

Previous WallDYN surface model

- Homogenous reaction layer + homogenous bulk
  - All erosion & deposition occurs homogenously in reaction layer
  - Composition of reaction layer is variable, composition of bulk is fixed
  - Reaction layer width held fixed via exchange with bulk (Γ^{EXCH})
  - Assume that trapped hydrogen does not affect sputtering rates
  - Physical sputtering and D-C chemical erosion included
- 1 Differential equation for areal density of each element in reaction layer:

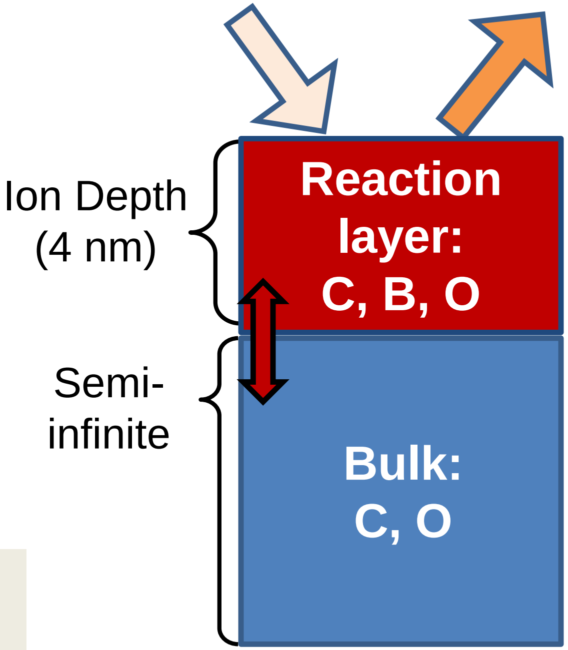
$$\frac{d}{dt}\left(\sigma_{wall,elem}^{REACTION}\right) = \Gamma_{wall,elem}^{IN}(t) - \Gamma_{wall,elem}^{REFL}(t) - \sum_{proj} \Gamma_{wall,elem}^{SPUT,proj}(t) - \Gamma_{wall,elem}^{EVAP}(t) \pm \Gamma_{wall,elem}^{EXCH}(t)$$

<u>Incident fluxes:</u>

- Constant D+, D-CX fluxes
- Energy-resolved redeposited impurity fluxes

<u>Outgoing fluxes:</u>

- Eroded impurity fluxes
- Reflected impurity fluxes
- Evaporated fluxes



Well suited for surfaces > 1 μm

New WallDYN “thin film” surface model

- The use of thin films for conditioning introduces an important new length scale in the system
  - Thin film width = Reaction layer width + Reservoir layer width
  - Composition of reservoir layer is variable
  - Reservoir width is dynamic
    - Net deposition → Reservoir grows
    - Net erosion → Reservoir shrinks
  - Reaction layer width held fixed via exchange with reservoir (Γ^{EXCH}), then bulk once reservoir is depleted
- 2 Differential equations for areal density of each element (1 for reaction layer, 1 for reservoir layer):

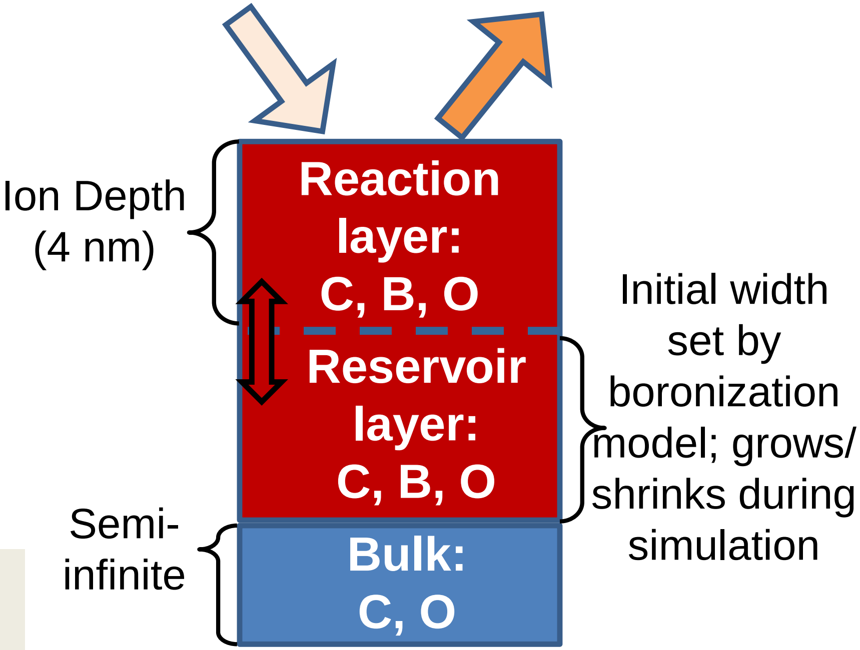
$$\frac{d}{dt}(\sigma^{REACTION}_{wall,elem}) = \Gamma^{IN}_{wall,elem}(t) - \Gamma^{REFL}_{wall,elem}(t) - \sum_{proj}\Gamma^{SPUT,proj}_{wall,elem}(t) - \Gamma^{EVAP}_{wall,elem}(t) \pm \Gamma^{EXCH}_{wall,elem}(t)$$

Incident fluxes:

- Constant D+, D-CX fluxes
- Energy-resolved redeposited impurity fluxes

Outgoing fluxes:

- Eroded impurity fluxes
- Reflected impurity fluxes
- Evaporated fluxes



Ion Depth (4 nm)

Reaction layer: C, B, O

Reservoir layer: C, B, O

Bulk: C, O

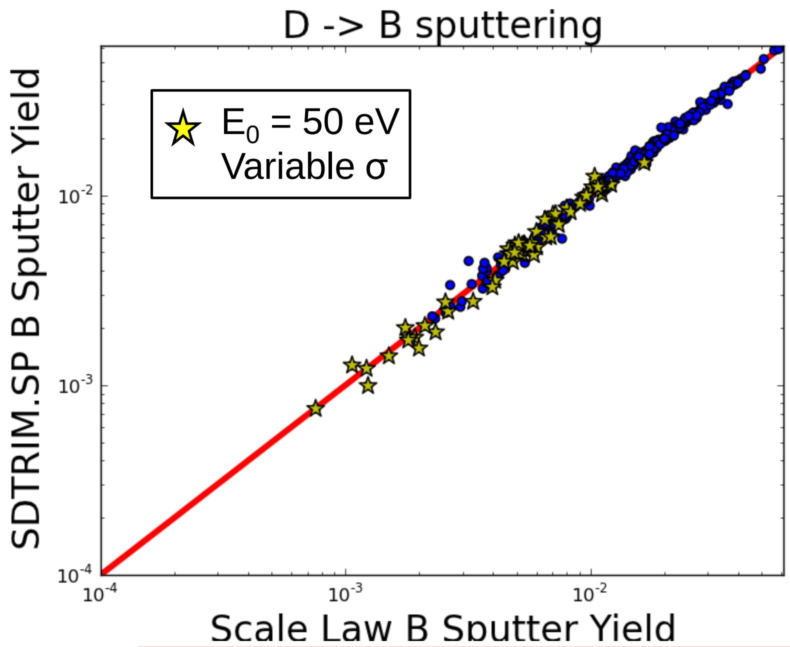
Semi-infinite

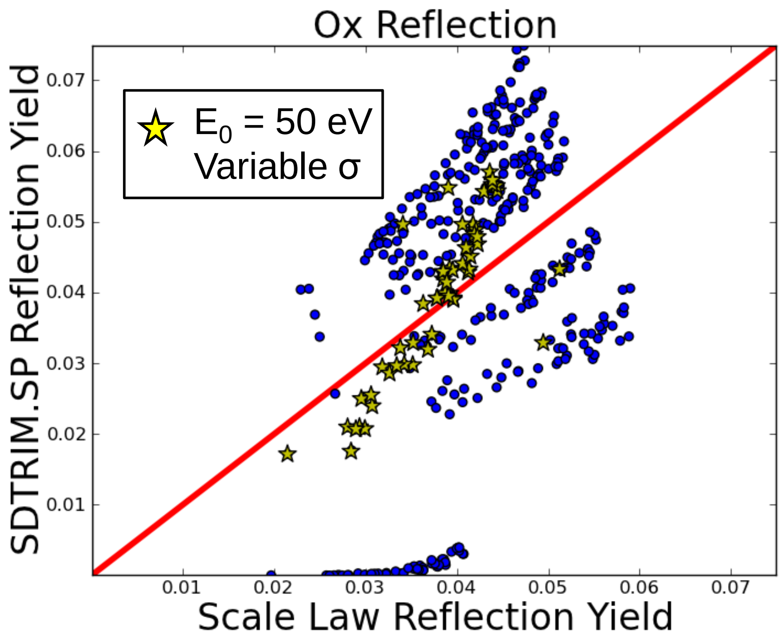
Initial width set by boronization model; grows/shrinks during simulation

$$\frac{d}{dt}(\sigma^{RESERVOIR}_{wall,elem}) = \mp\Gamma^{EXCH}_{wall,elem}(t)$$

WallDYN parameterizes mixed material sputtering and reflection with SDTRIM.SP

- SDTRIM.SP varied over projectile/energy/surface composition (1600+ runs)





$$Y_{sput}^{FIT} = \boxed{Q * s_n(E_0/E_{TF}) * (1-(E_{th}/E_0)^{2/3}) * (1-E_{th}/E_0)^2 *} \boxed{(1 + \Sigma_i\, \sigma_i * a_i)}$$

Bohdansky formula

Composition dependence

$$Y_{refl}^{FIT} = \rho_{refl} * E_0^{\alpha} * \boxed{(1 + \Sigma_i\, \sigma_i * b_i)}$$

Composition dependence

σ_i = areal density of element i

Fit parameters: Q, E_{th}, a_C, a_{Li}, a_O

σ_i = areal density of element i

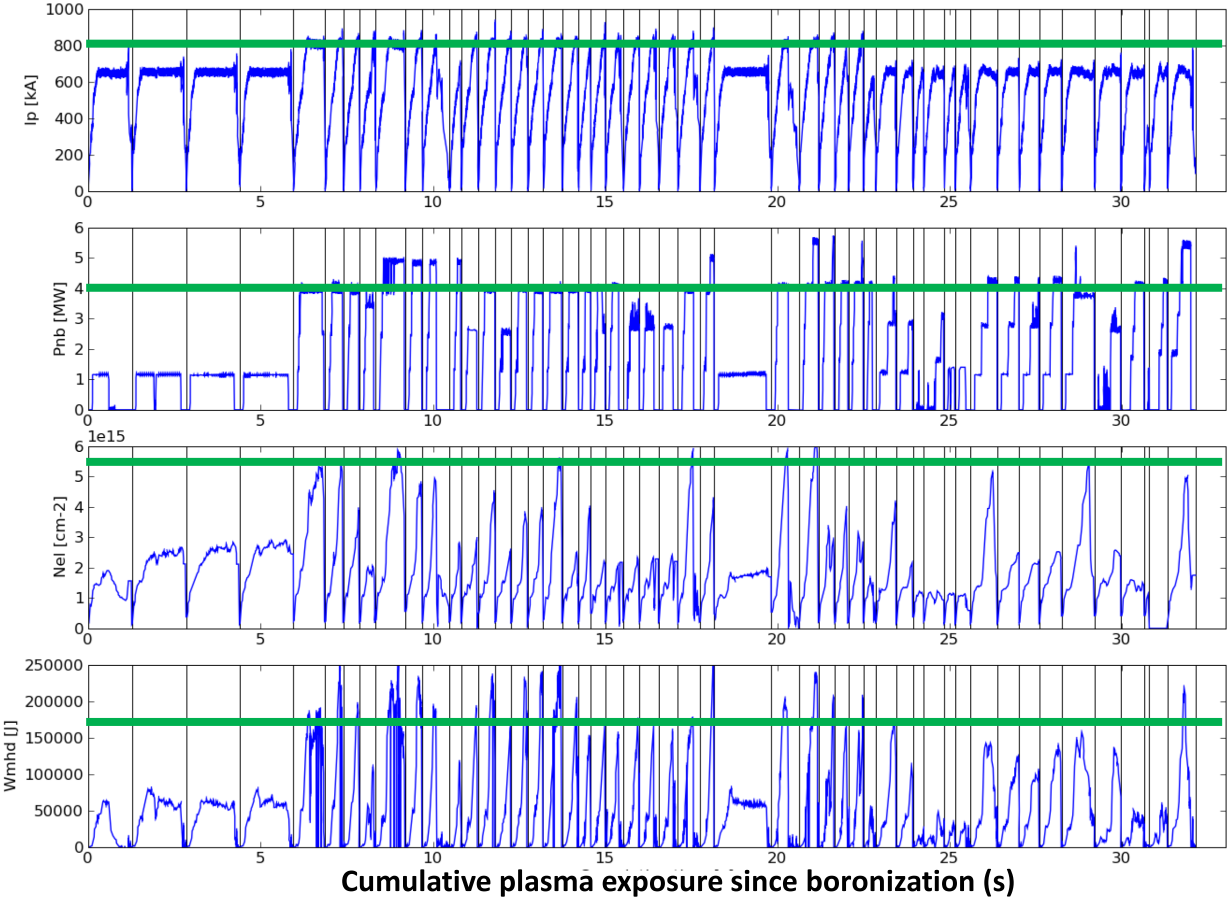
Fit parameters: ρ_{refl}, α, b_C, b_{Li}, b_O

PLASMA MODEL

Campaign-relevant plasma parameters chosen for plasma model

- NSTX-U shots were highly varied, transient, and not always controlled
  - Still, “peak” performance, expected to be primary driver of erosion, can be decently represented by a medium-performance NSTX H-mode proxy

Plasma Operations following Boronization #8 (203953-204011)



Plasma Current

Proxy (129015): 0.80 MA

NBI Power

Proxy (129015): 4 MW

Line-avg Density

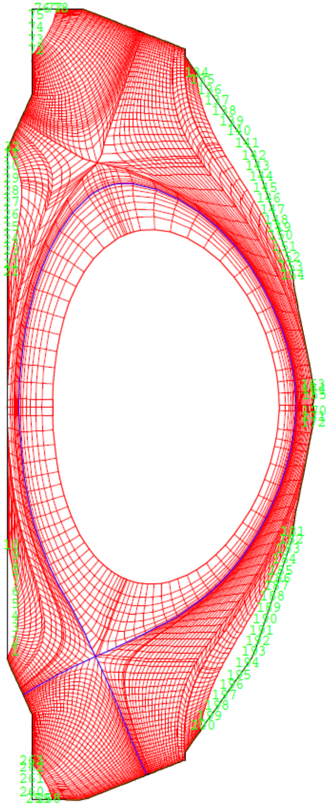
Proxy (129015): 5.5e15 cm^{-2}

Stored Energy

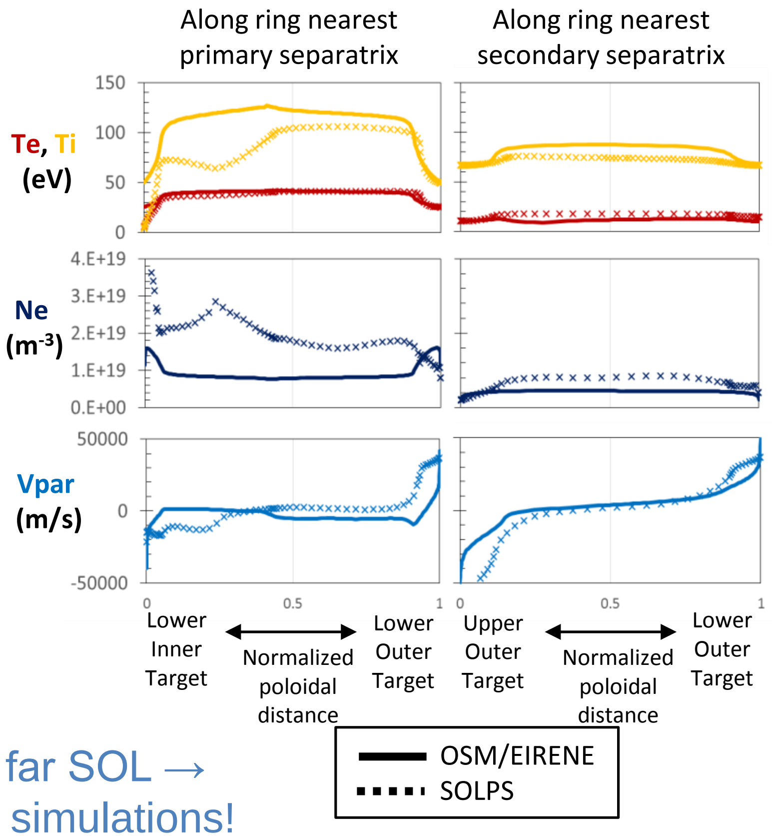
Proxy (129015): 160 kJ

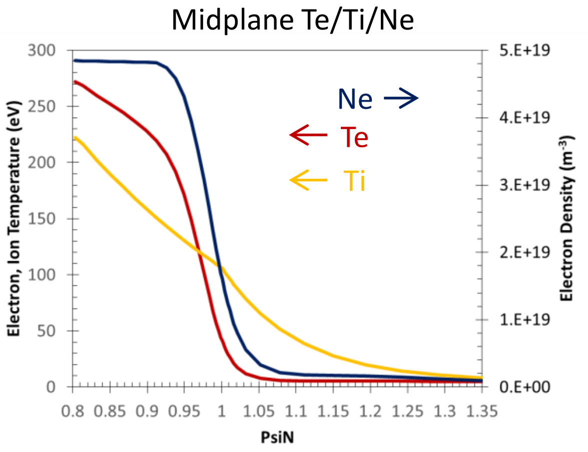
Extended grid SOL plasma solution generated with two-fluid onion skin solver

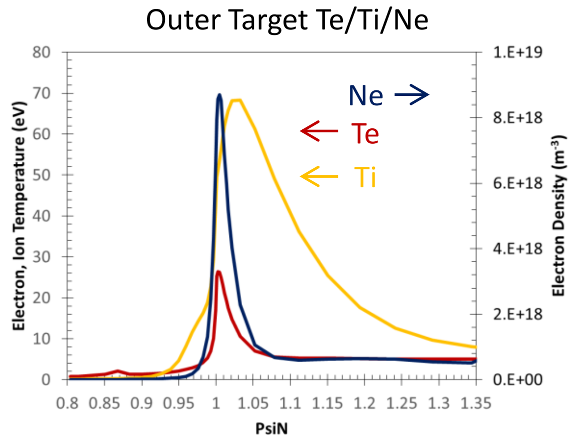
- OSM/EIRENE applied to boundary conditions of validated SOLPS reconstruction of boronized NSTX H-Mode [Canik PoP 2011]
  - No NSTX-U probe data available for direct reconstruction of discharges



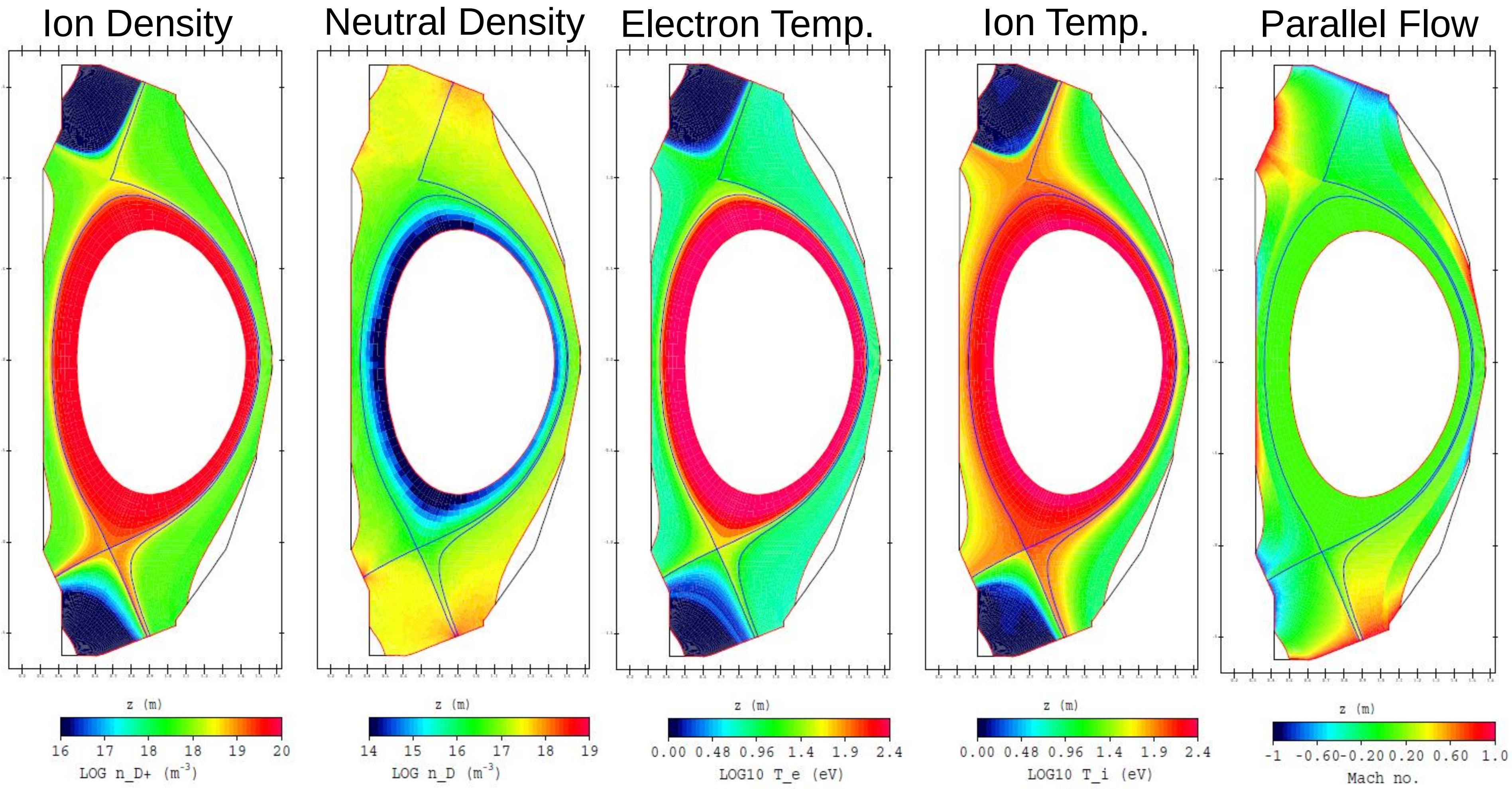
“Extended” grid fills far SOL → critical for migration simulations!







OSM/EIRENE edge plasma background generated for NSTX-U



Ion Density

Neutral Density

Electron Temp.

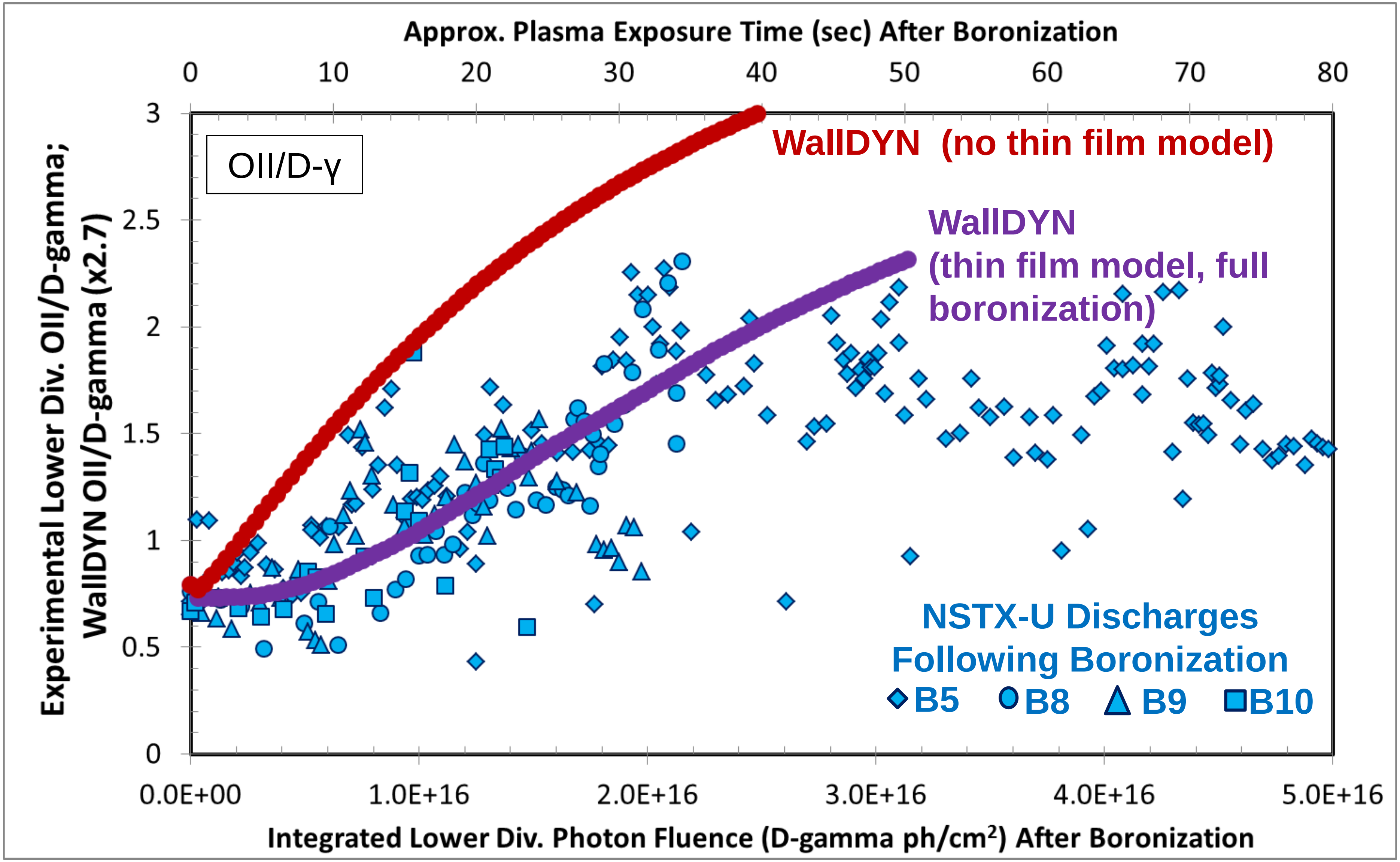
Ion Temp.

Parallel Flow

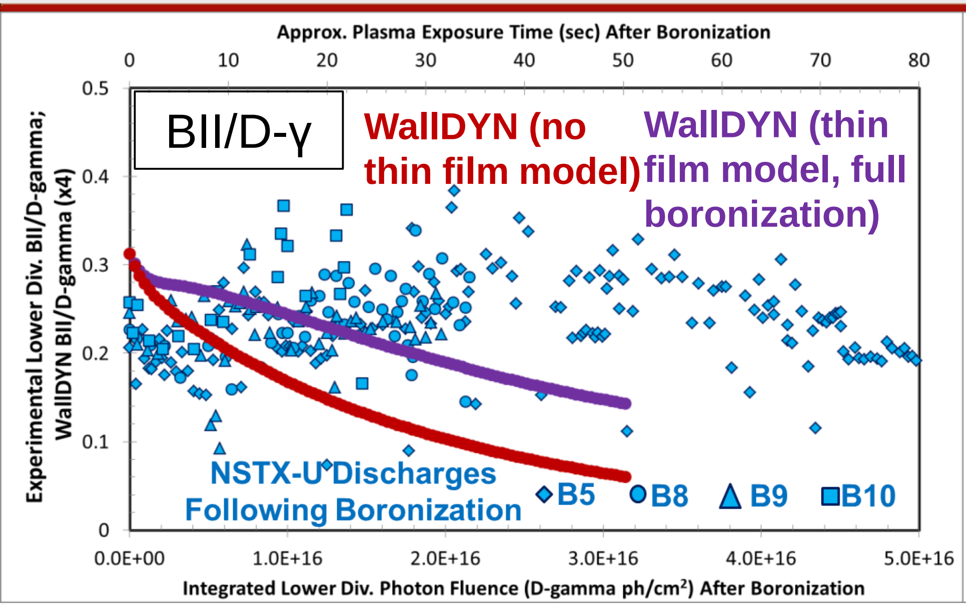
- High strike point density/temperature, large radial gradients (H-Mode like)
- No external flow/pinch applied

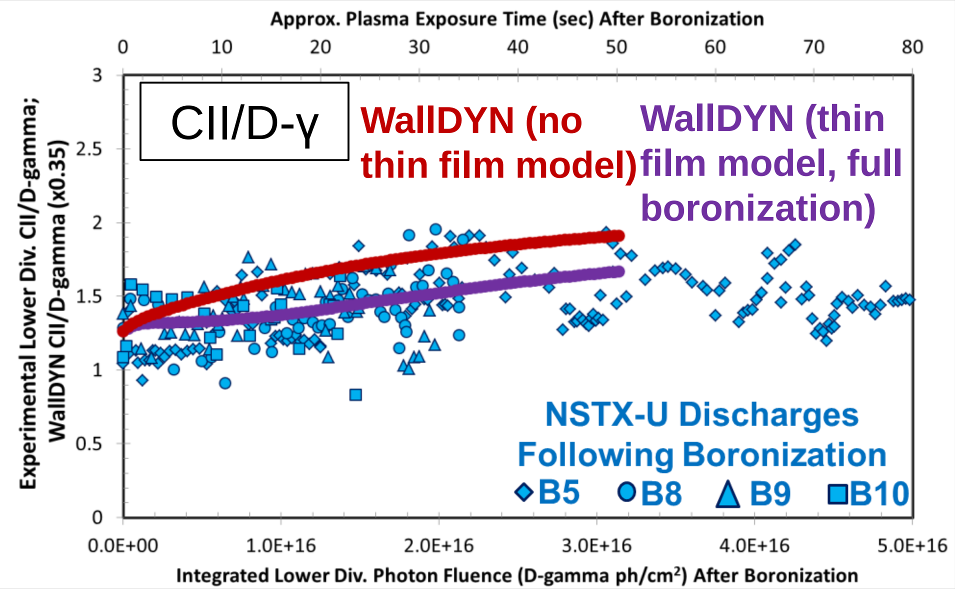
RESULTS

Results: agreement with OII emission trends greatly improved with thin film model



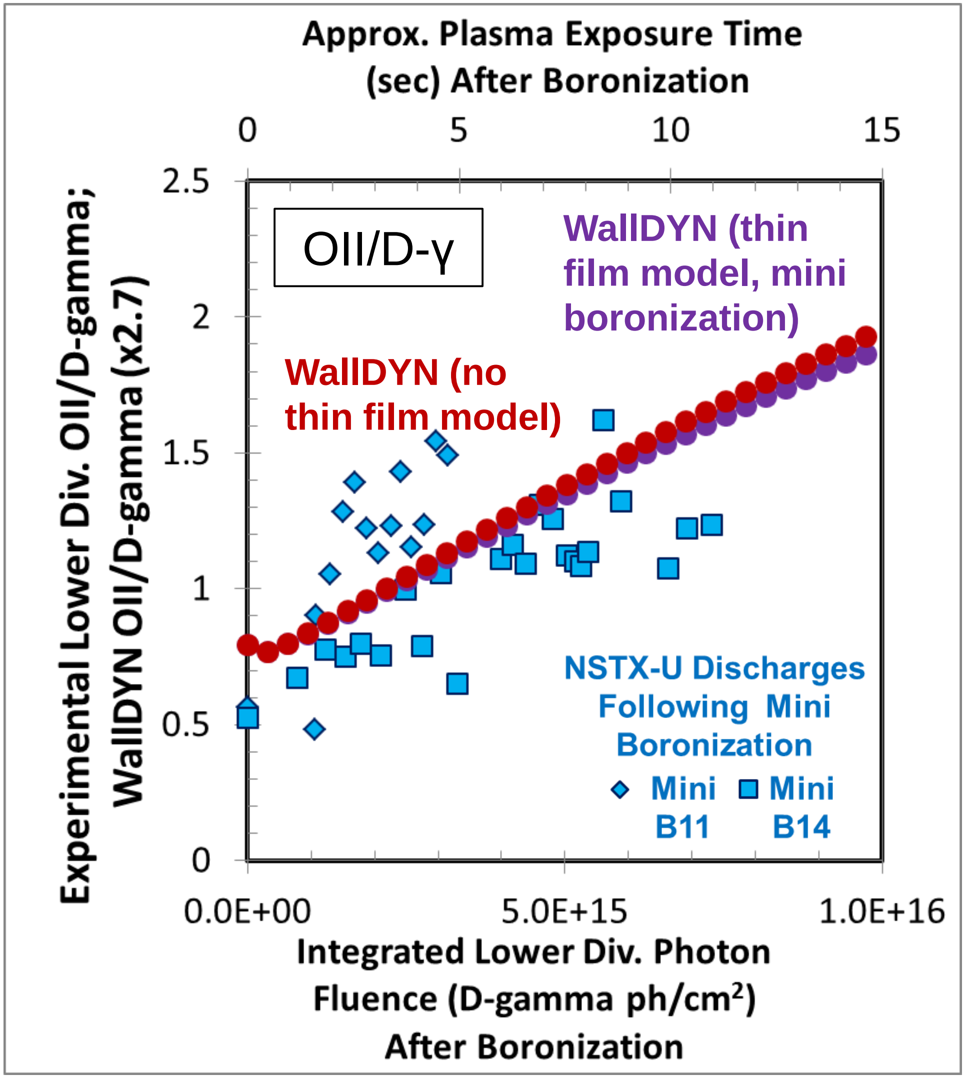
Results: agreement with BII, CII emission trends slightly improved with thin film model





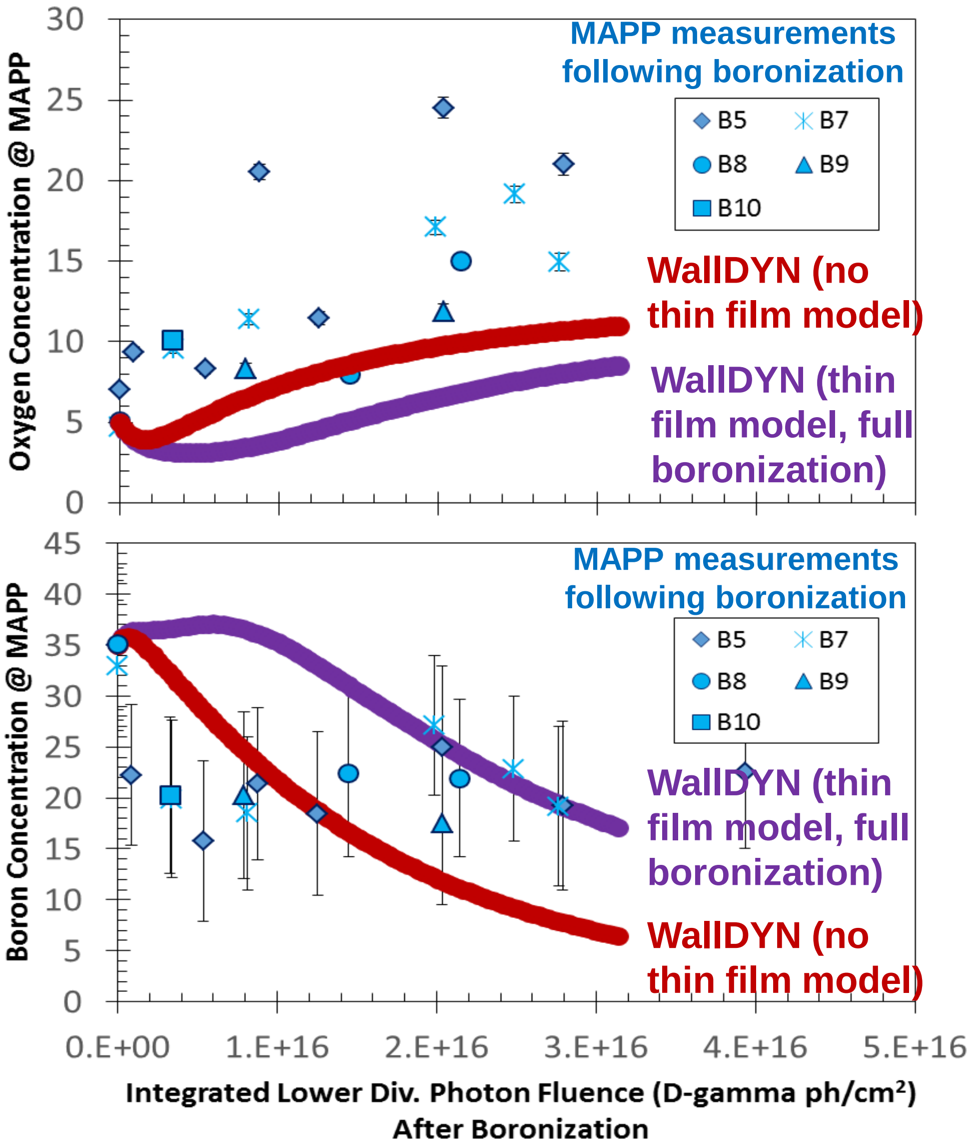
- Thin film model brings WallDYN into good agreement with experimental oxygen emission trends following full boronizations
- No experimental trend in carbon emission following boronization
  - Good agreement with both WallDYN models
- No experimental trend in boron emission following boronization
  - Poor agreement with both WallDYN models
  - Reason for continued disagreement is under investigation

Results: agreement with mini boronization emission trends similar with either model



- Thin film WallDYN model capable of differentiating between full and mini boronizations
  - Captures faster rise in impurity influx following mini boronization
- Both model and experiment show degradation of mini boronization coating on time scale of ~ 1 run day (15 sec plasma exposure)
- For mini boronization, thin film WallDYN model is nearly identical to old WallDYN model
  - Makes sense, because boron film applied to divertor (~30 A) is thinner than reaction layer (ion penetration depth ≈ 40 A)

Results: surface concentration evolution during simulations



- Both WallDYN models underestimate the rise in oxygen surface composition observed in MAPP
- Surface boron agreement inconclusive

- Models do not take into account chemical state of surface
  - e.g. B-O vs. B-B vs. B-C bonds
  - May be important!

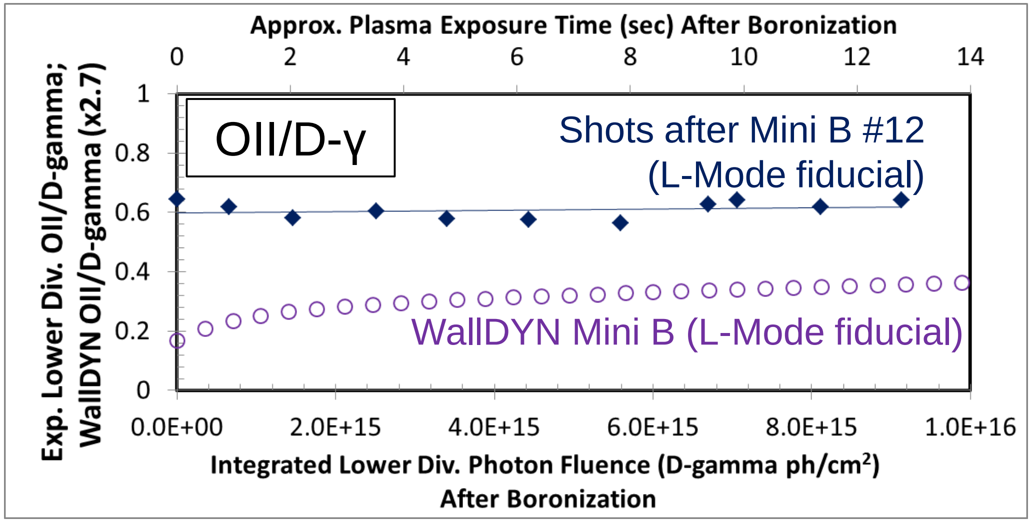
For more B/C/O surface discussion see:

F. Bedoya JO4.10 Tue PM

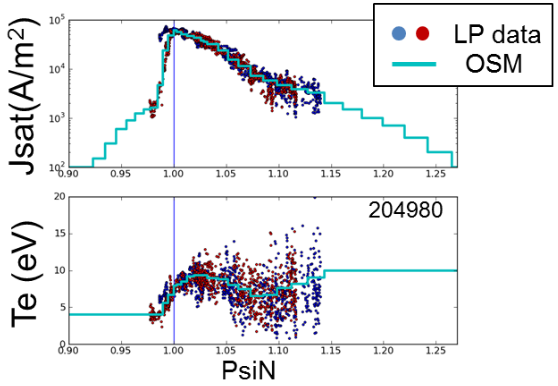
H. Schamis PP11.57 Wed PM

Closer look: No evolution observed after exposure to L-Mode fiducial only

- Mini Boronization #12: 11 consecutive L-Mode fiducial discharges
  - Limited Langmuir probe data available for late-campaign L-Mode fiducial
  - Direct comparison is possible
- No oxygen impurity emission evolution is observed over the course of the run day
  - MAPP also shows similar surface oxygen concentration before + after
- Model reproduces general trend after 2nd discharge
  - OII/D-γ magnitude low

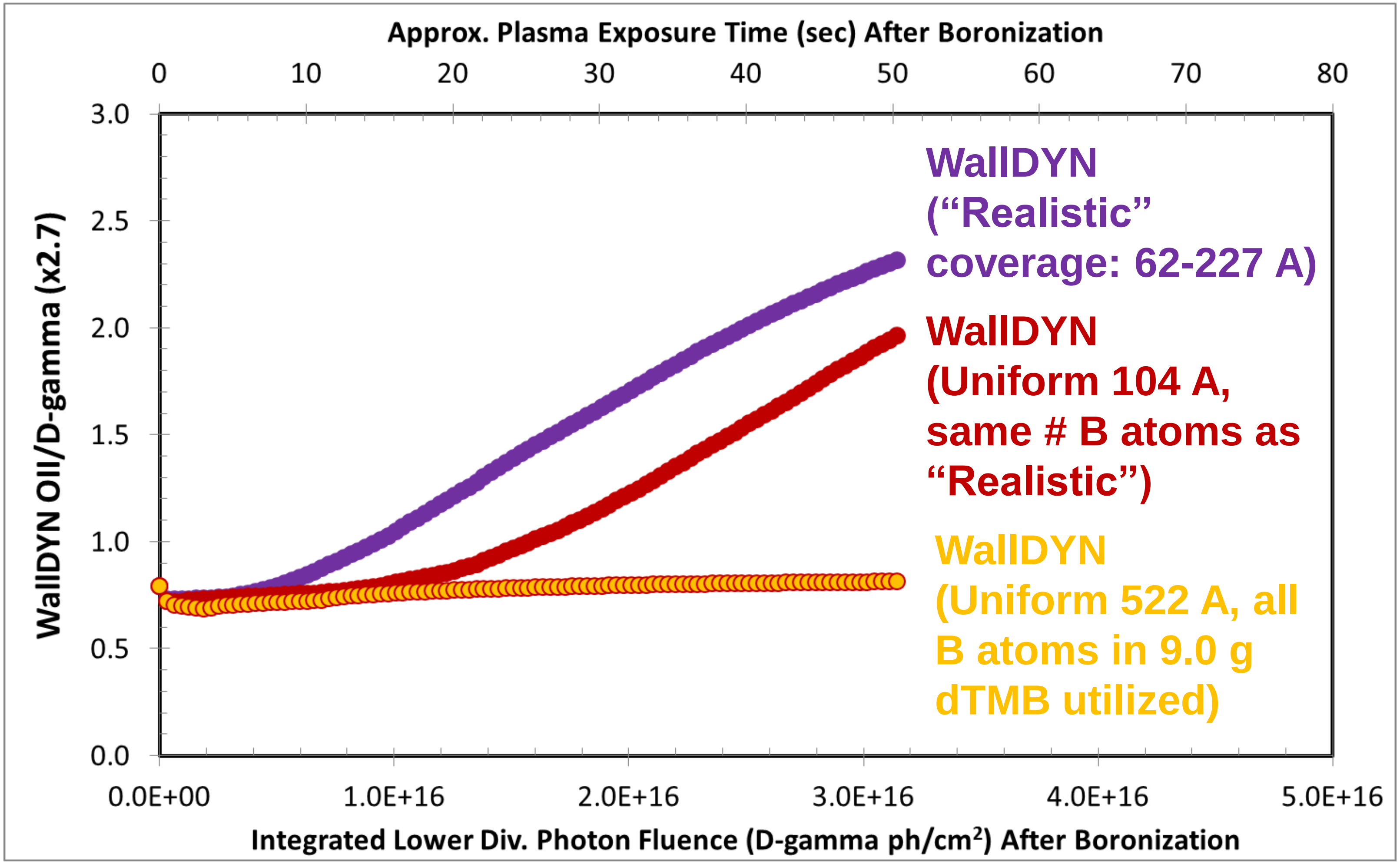


- Highly likely that WallDYN L-Mode fiducial model does not fully capture evolution driven by higher-power general purpose L-Modes
  - Not enough H-Modes in campaign to explain general OII evolution otherwise



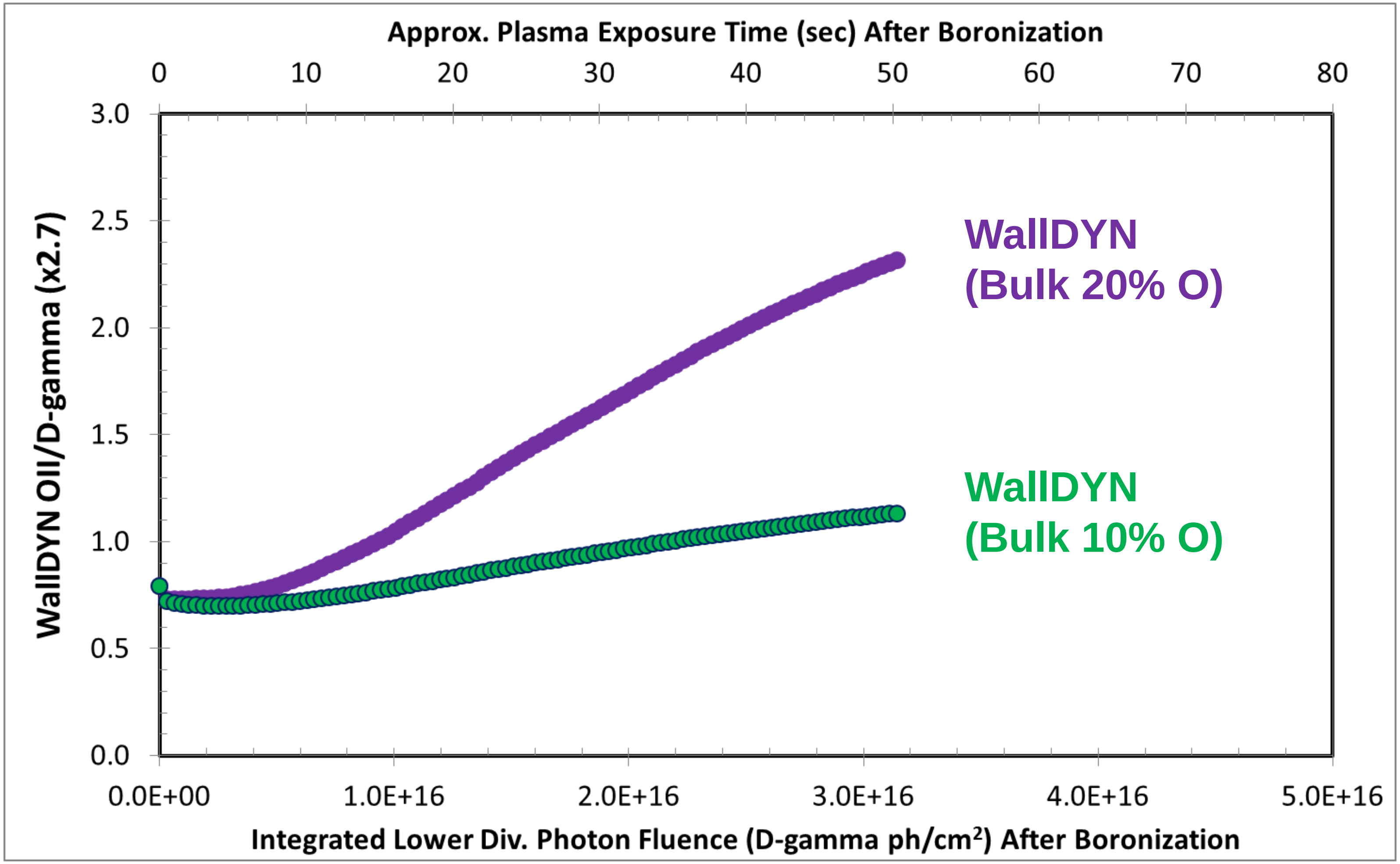
PREDICTIONS

Effect of more uniform boron coverage on oxygen evolution (*aka more GDC electrodes*)



- Uniformity of boron coatings is controlled by properties of He glow discharge and the number of anodes

Effect of lower bulk oxygen concentration on oxygen evolution (*aka better bakeout*)



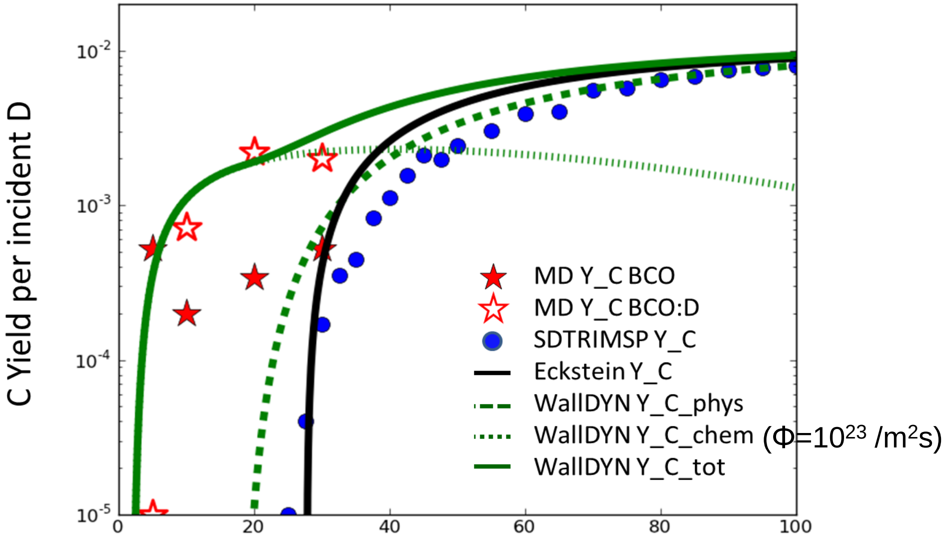
- Bulk oxygen content is typically controlled by pre-campaign conditioning (bakeout, etc.)

CONCLUSIONS

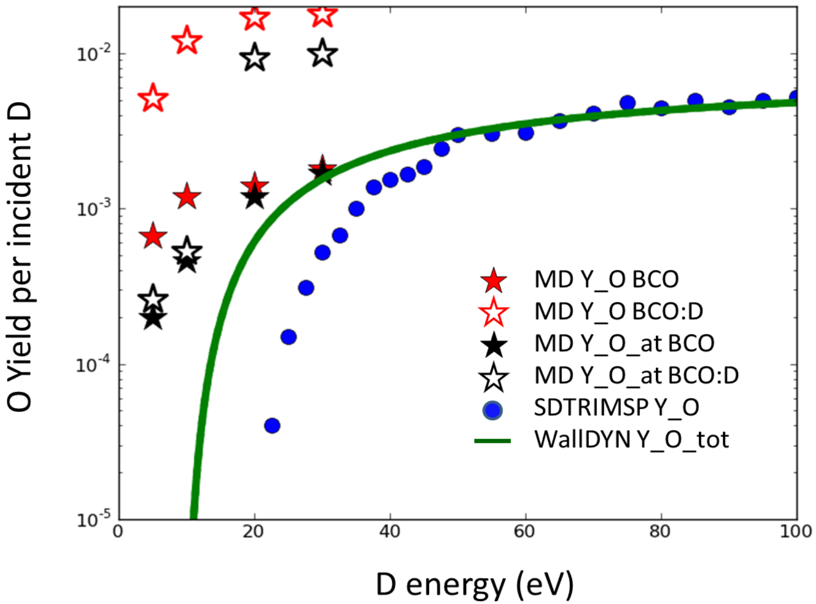
- The integrated material migration model WallDYN has been improved through comparison to NSTX-U experimental data
  - WallDYN surface model modified to incorporate finite thin films, as used in wall conditioning
  - Model reproduces impurity emission trends observed following boronization in NSTX-U
    - ✓ Boronization suppresses OII emission
    - ✓ OII emission increases with plasma exposure
    - ✓ OII emission increases faster following a mini boronization
  - Model qualitatively reproduces surface composition evolution observed with MAPP
  - New multi-layer surface model improves agreement with measurables

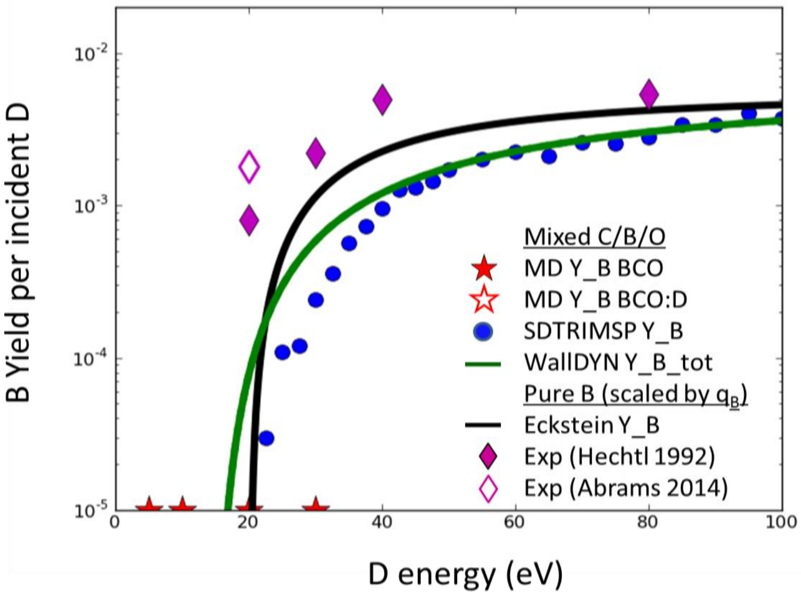
- Future work: Full-scale model validation
  - Requires repeatable research-grade plasma scenario
  - Requires absolutely-calibrated spectroscopic diagnostics
  - Requires well-constrained SOL plasma reconstruction
    - ▪ Independent plasma flow diagnostic highly desirable
  - Requires independent validation of mixed-material sputtering model

Notable area for model improvement: High-fidelity low-energy sputtering yields



($\Phi=10^{23}$ /m^{2}s)





WallDYN/TRIM vs. Molecular Dynamics

D -> 60%C, 20%B, 20%O at normal incidence

MD: [J. Dominguez-Gutierrez JAP 2017]

- Y_C well fit when including flux-dependent chem. erosion model
- Y_O much higher than model
- Y_B much lower than model