NSTX-U

Supported by U.S. DEPARTMENT OF ENERGY | Office of Science

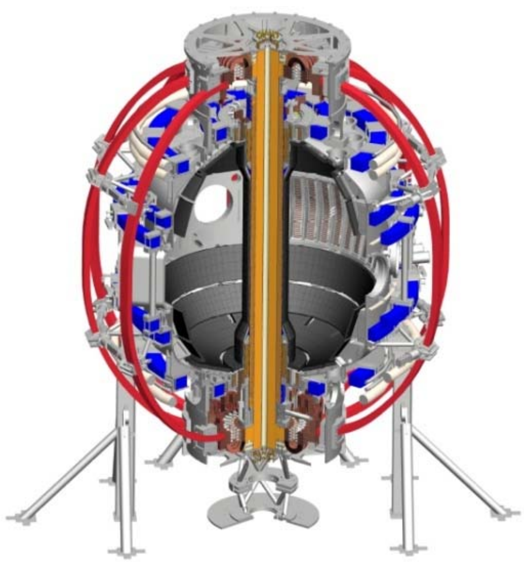
Erosion and re-deposition of lithium and boron coatings under high-flux plasma bombardment

Tyler Abrams

M.A. Jaworski, R. Kaita, J.H. Nichols, D.P. Stotler, G. De Temmerman, M.A. van den Berg, H.J. van der Meiden, T.W. Morgan

APS-DPP Meeting
New Orleans, LA
October 29, 2014

Coll of Wm & Mary
Columbia U
CompX
General Atomics
FIU
INL
Johns Hopkins U
LANL
LLNL
Lodestar
MIT
Lehigh U
Nova Photonics
ORNL
PPPL
Princeton U
Purdue U
SNL
Think Tank, Inc.
UC Davis
UC Irvine
UCLA
UCSD
U Colorado
U Illinois
U Maryland
U Rochester
U Tennessee
U Tulsa
U Washington
U Wisconsin
X Science LLC

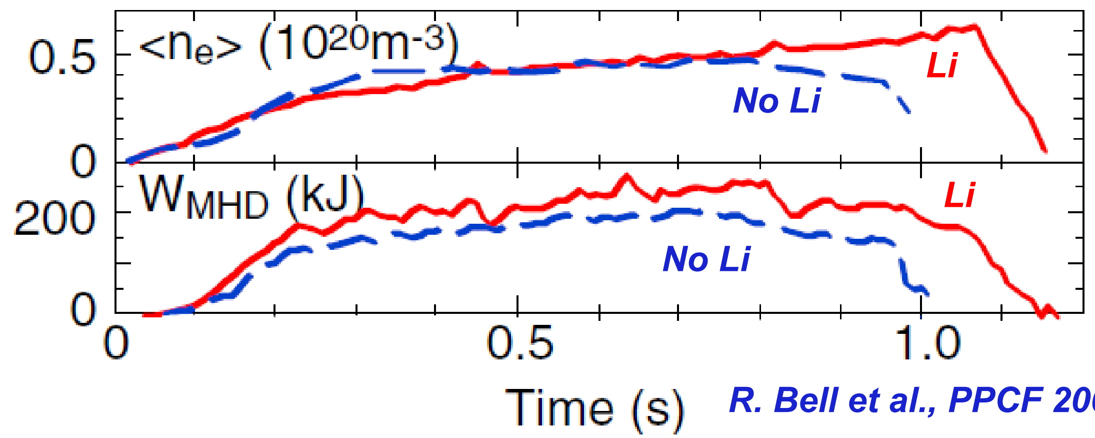


Culham Sci Ctr
York U
Chubu U
Fukui U
Hiroshima U
Hyogo U
Kyoto U
Kyushu U
Kyushu Tokai U
NIFS
Niigata U
U Tokyo
JAEA
Inst for Nucl Res, Kiev
Ioffe Inst
TRINITI
Chonbuk Natl U
NFRI
KAIST
POSTECH
Seoul Natl U
ASIPP
CIEMAT
FOM Inst DIFFER
ENEA, Frascati
CEA, Cadarache
IPP, Jülich
IPP, Garching
ASCR, Czech Rep

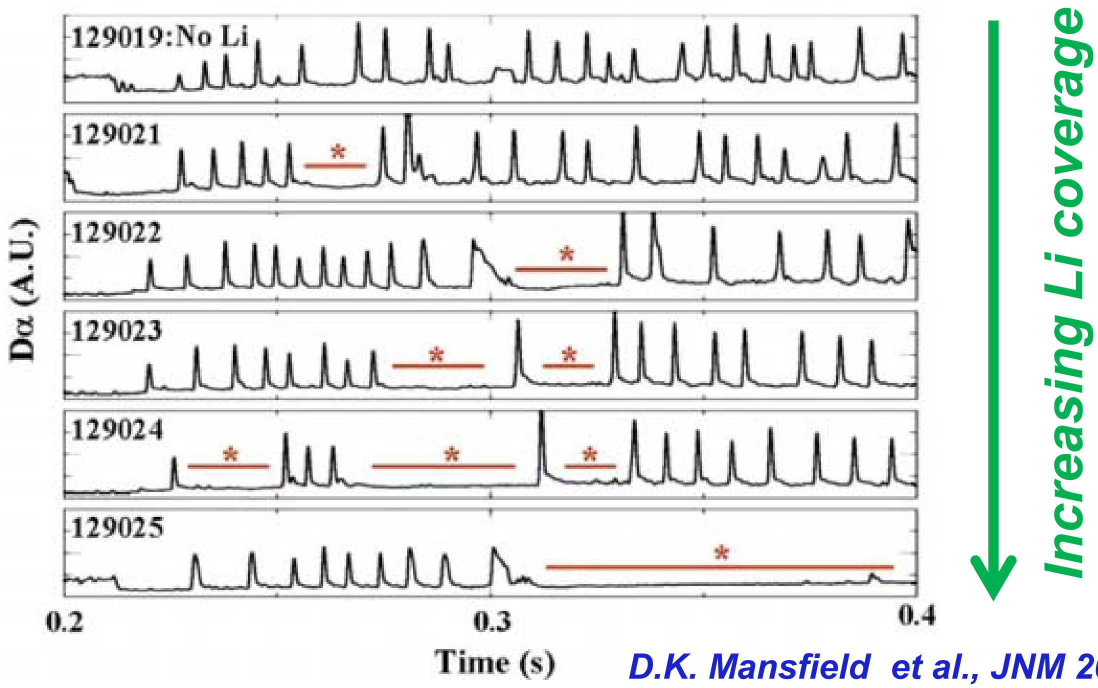
Lithium improves plasma performance and protects underlying substrates

- Improved performance:
  - Increased n_e, W_{MHD}
  - ELM reduction
- Li protects even fragile porous substrates from high heat fluxes[a,b]
- Liquid Li is an alternative to W for a DEMO PFC
  - Self-healing under plasma bombardment
  - Eroded material can be replenished by flow

Li Films in NSTX



R. Bell et al., PPCF 2009



D.K. Mansfield et al., JNM 2009

[a] *G. Mazzitelli et al., FED 2010*
[b] *T. Abrams et al., JNM 2013*

Previous results on flow-flux devices suggest Li erosion may be unacceptably high at elevated temperatures

- Li erosion rate scales with temperature
  - Evaporation (Langmuir Law)
  - T-dependent sputtering (PISCES-B, IIAX, DIII-D)

- Thermal-spike model[a]:

$$Y(T_{Li}) = \frac{A}{\sqrt{kT_{Li} + B}} \exp\left(\frac{-1.59\ \text{eV}}{\sqrt{kT_{Li} + B}}\right)$$

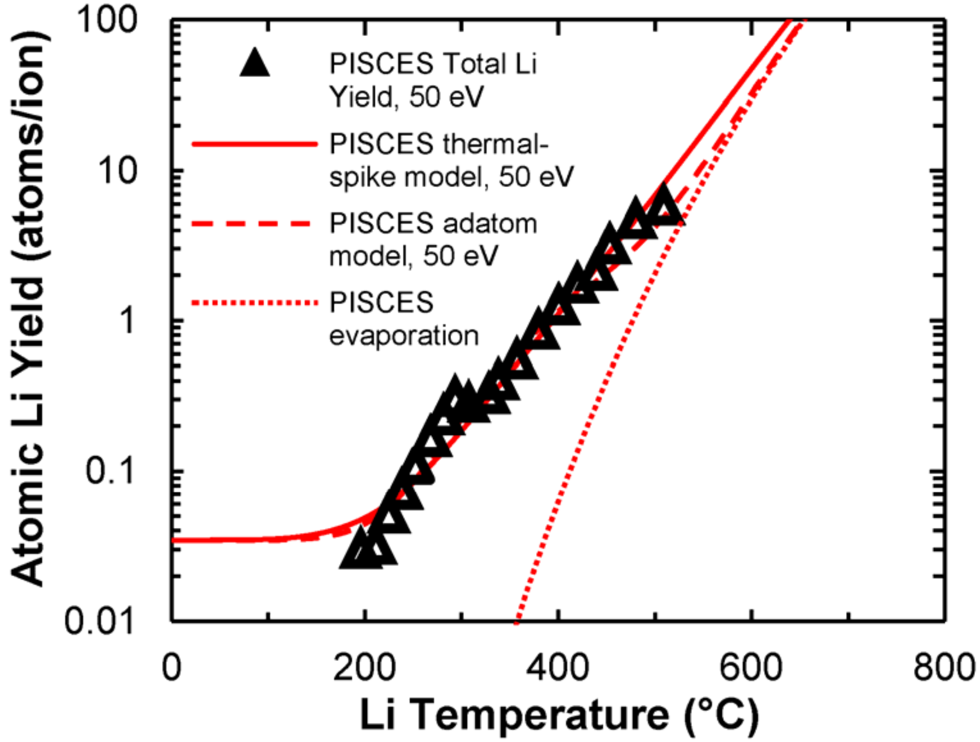
A,B: Fitting parameters
k: Boltzmann's constant

- Adatom-sublimation model[b]:

$$Y(T_{Li}) = \frac{Y_{ad}}{1 + A \exp\left(\frac{E_{eff}}{kT_{Li}}\right)}$$

Y_{ad}, A, E_{eff}: Fitting Parameters

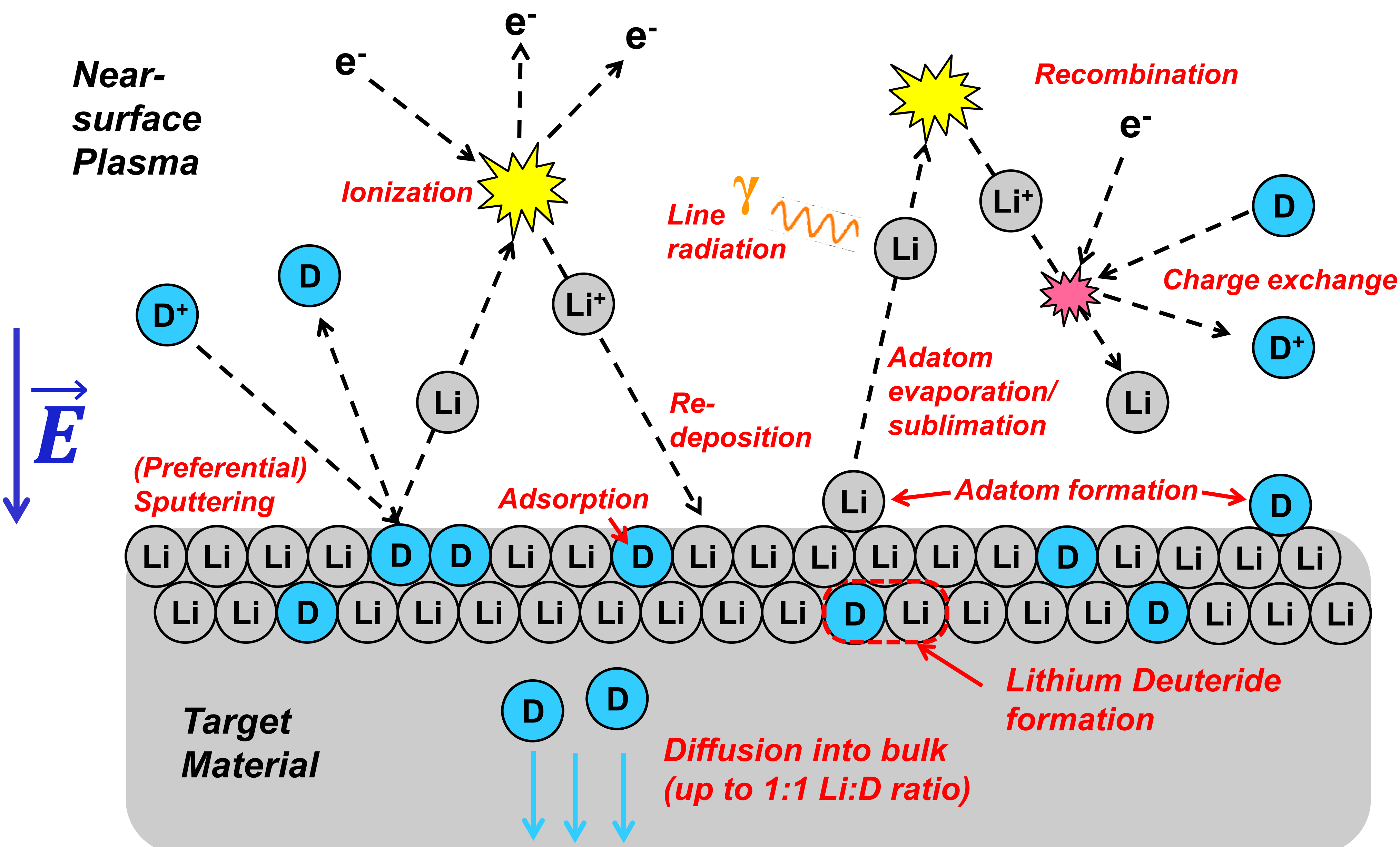
Atomic Li Yield vs. Li Temperature Measured on PISCES-B



R.P. Doerner et al., JNM 2001

[a]*J.P. Allain et al., Phys Rev B 2007*
[b]*R.P. Doerner et al., J. App. Phys. 2004*

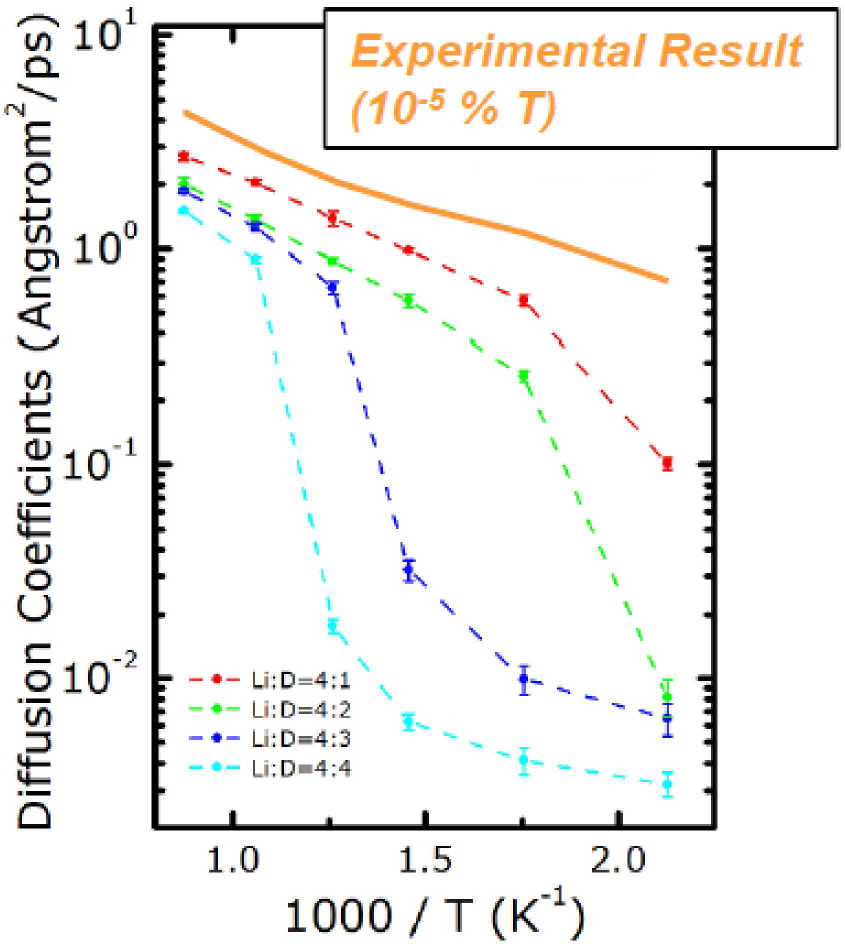
Many processes are involved in the D-Li PMI



D diffusion in Li has been characterized using molecular dynamics (MD) simulations

- Recent MD simulations[a] have calculated D diffusivity in Li vs. temperature and D/Li concentration (**β**)

D diffusivity in Li



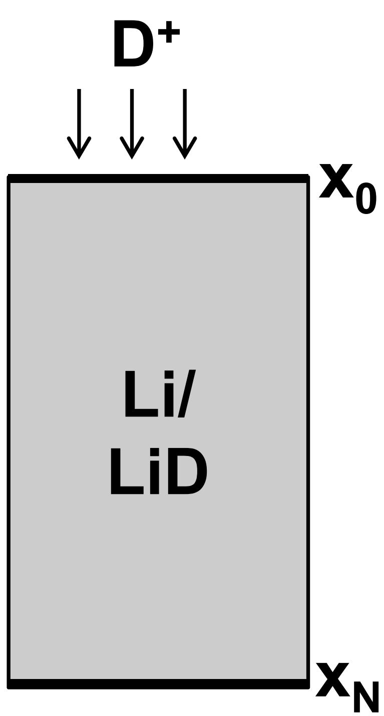
- Diffusion coefficients decrease strongly vs. D/Li concentrations
- Evidence of LiD solidification for 100% LiD
  - LiD melting temp: 965 K ($1000/T_{melt} = 1.04$)

[a]*M. Chen and E.A. Carter, Nuc. Fusion, in prep.*
[b]*H. Moriyama et al., JNM 1992*

Time evolution of Li:D concentration can be determined for any plasma/surface conditions

- Solve 1-D diffusion equation with time and space-dependent diffusion coefficients
- D assumed implanted uniformly in top 5 nm of material

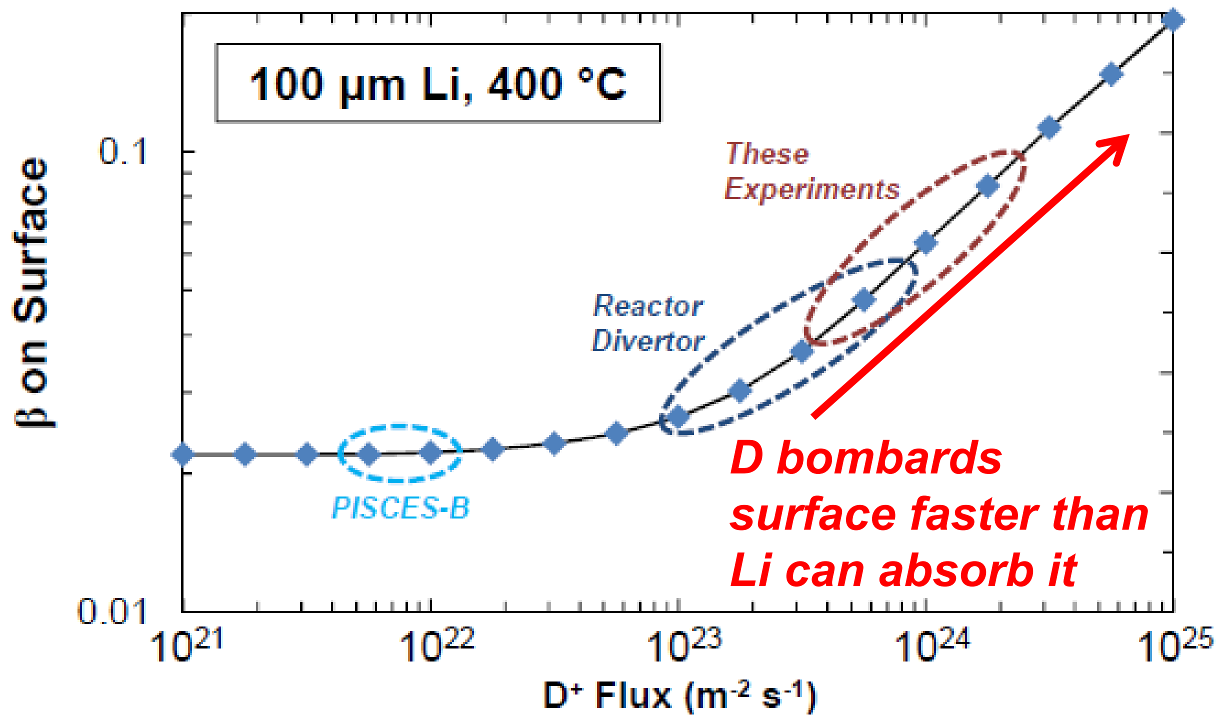
$$\frac{d\beta(x,t)}{dt} = D(\beta)\frac{d^2\beta(x,t)}{dx^2}$$



$$\left.\frac{d\beta}{dx}\right|_{x_0} = 0$$

$$\left.\frac{d\beta}{dx}\right|_{x_N} = 0$$

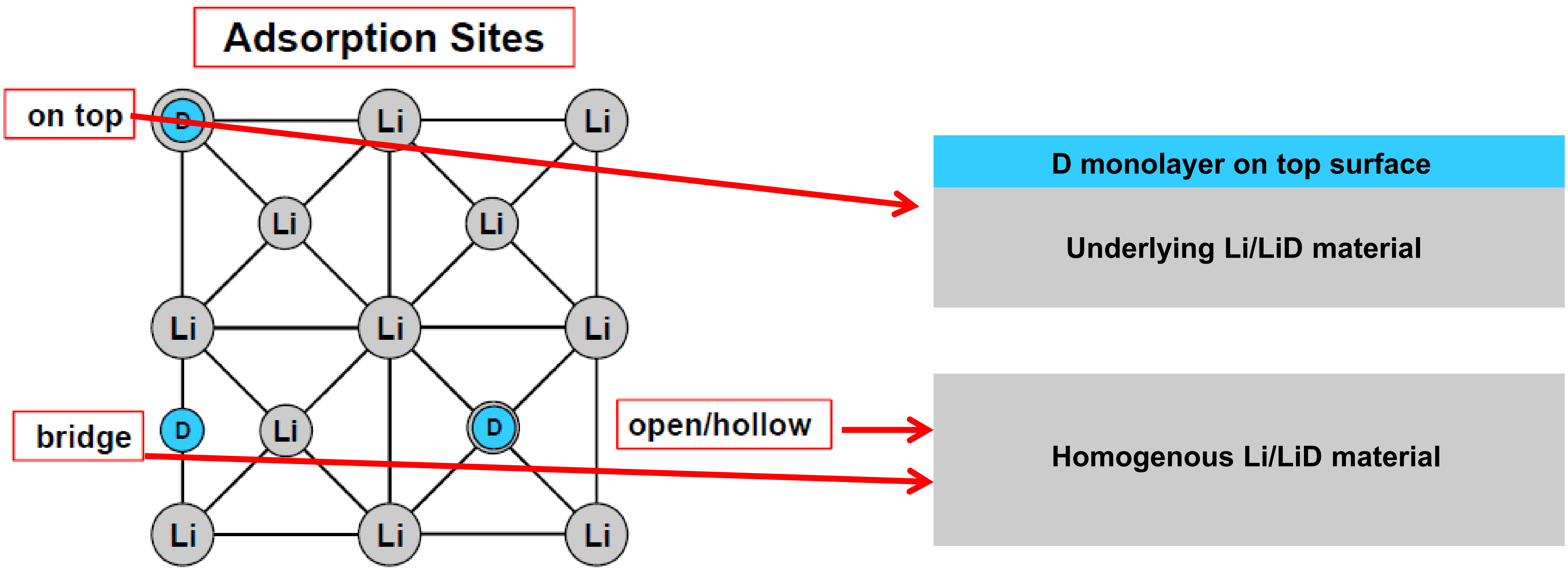
Surface D / Li concentration after D fluence of 10^{23} m^{-2}



How does D concentration on Li surface affect sputtering?

- D absorption reduces Li sputtering in two ways:
  - **Preferential sputtering**: less atoms available to sputter
  - **Chemistry**: SBE* is higher for LiD (2.26 eV) vs. Li (1.67 eV)

- D atoms can adsorb on a Li surface in several different sites
  - Motivates two different models of a Li/LiD surface



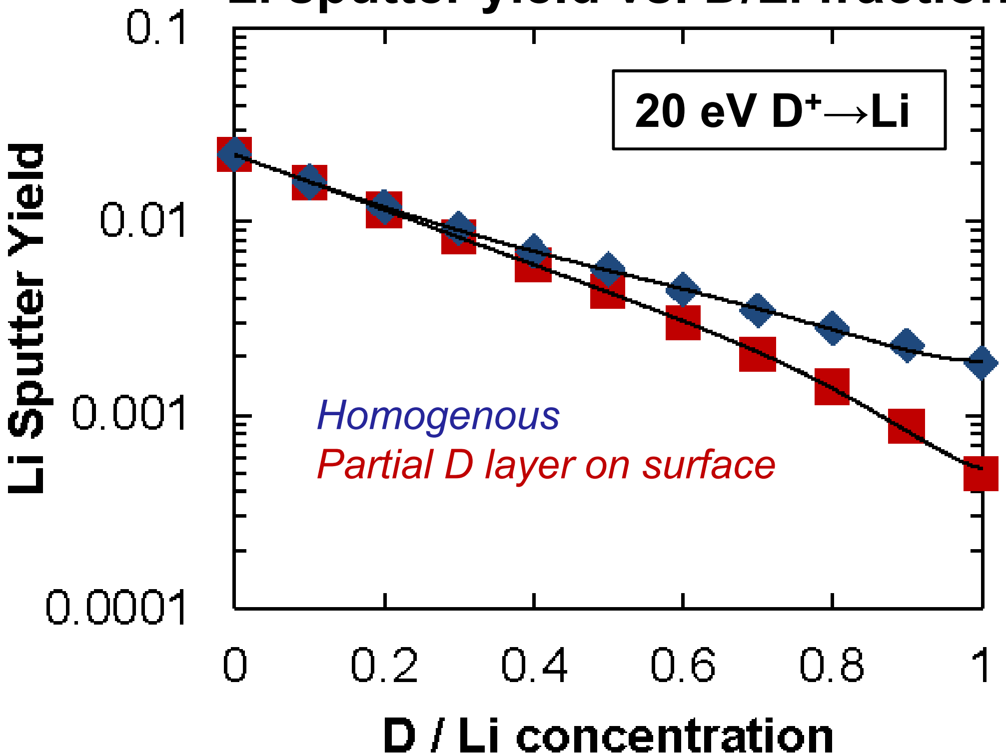
**Assumed equal to heat of sublimation*

Sputtering on a Li/LiD surface can be simulated with SDTrimSP binary collision approximation (BCA) code[a]

- Preferential sputtering is directly incorporated
- Chemical effects simulated by interpolation of SBEs:

$$\mathbf{SBE_{eff}} = (1-\beta)\mathbf{SBE_{Li}} + \beta\mathbf{SBE_{LiD}}$$

SDTrimSP simulations of Li sputter yield vs. D/Li fraction



- D impurities in Li results in **strong reduction of $Y_{D \rightarrow Li}$**
- Reduction for 100% LiD:
  - **~10x** in homogeous case
  - **~40x** w/ D monolayer on LiD surface
- Empirically fit $f(\beta)$

[a]A.Mutzke, R.Schneider, W.Eckstein, R.Dohmen, SDTrimSP Version 5.0. IPP Report 12/8, Garching, (2011)

Evaporation of LiD in suppressed relative to pure Li

- Li vapor pressure above Li/LiD mixtures is reduced relative to pure Li

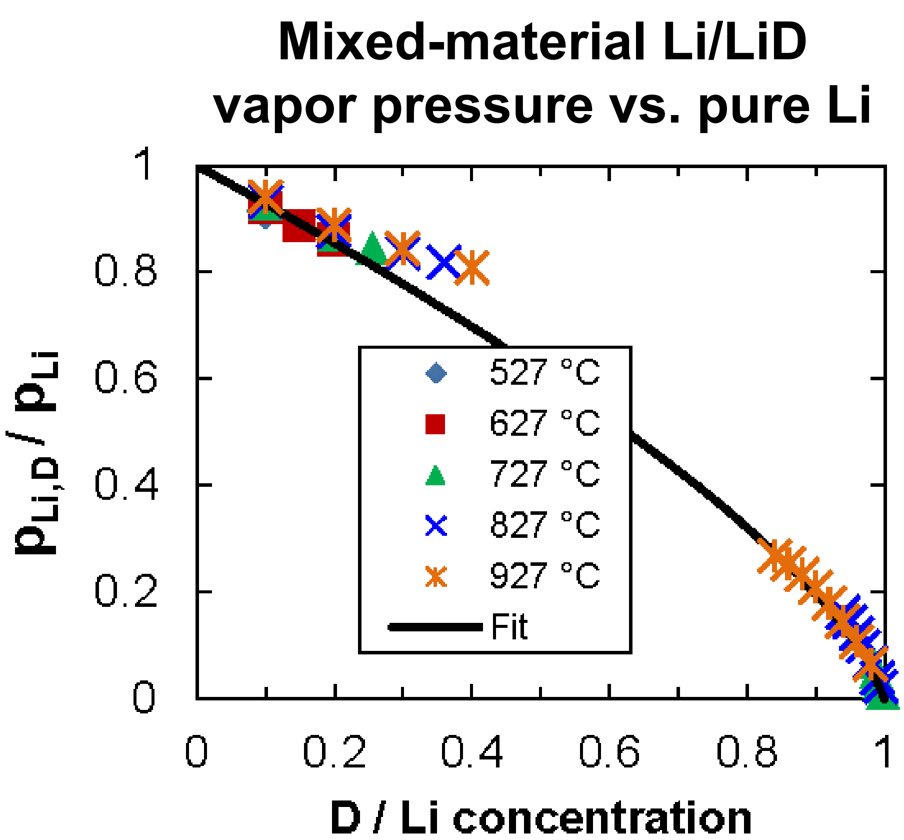
- Reduction factor is independent of temperature

$$\Gamma_{\text{evap}}(T_{Li}) = \frac{p_{Li,D}}{\sqrt{2\pi m_{Li} k T_{Li}}}$$

Γ_{evap}: Evaporative Li flux
p_{Li}: Li vapor pressure
m_{Li}: Li mass (6.941 amu)

- Empirical fit formula:

$$\frac{p_{Li,D}}{p_{Li}} = (1 - \beta)^{0.705}$$



E.E. Shpil'rain et al., 1987

Corrected Li erosion model is a function of Li temperature and D concentration in the Li

$$\Gamma_{Li}(T_{\mathrm{Li}},\beta,\Gamma_{D+}) = \Gamma_{D+}f(\beta)\left[\frac{Y_{\mathrm{coll}}}{3}+\frac{Y_{ad}}{1+A\exp\left(\frac{E_{eff}}{k_B T_{Li}}\right)}\right]+\frac{p(T_{Li},\beta)}{\sqrt{2\pi m_{Li}k_B T_{Li}}}$$

Total Li erosion ($m^{-2}\ s^{-1}$)

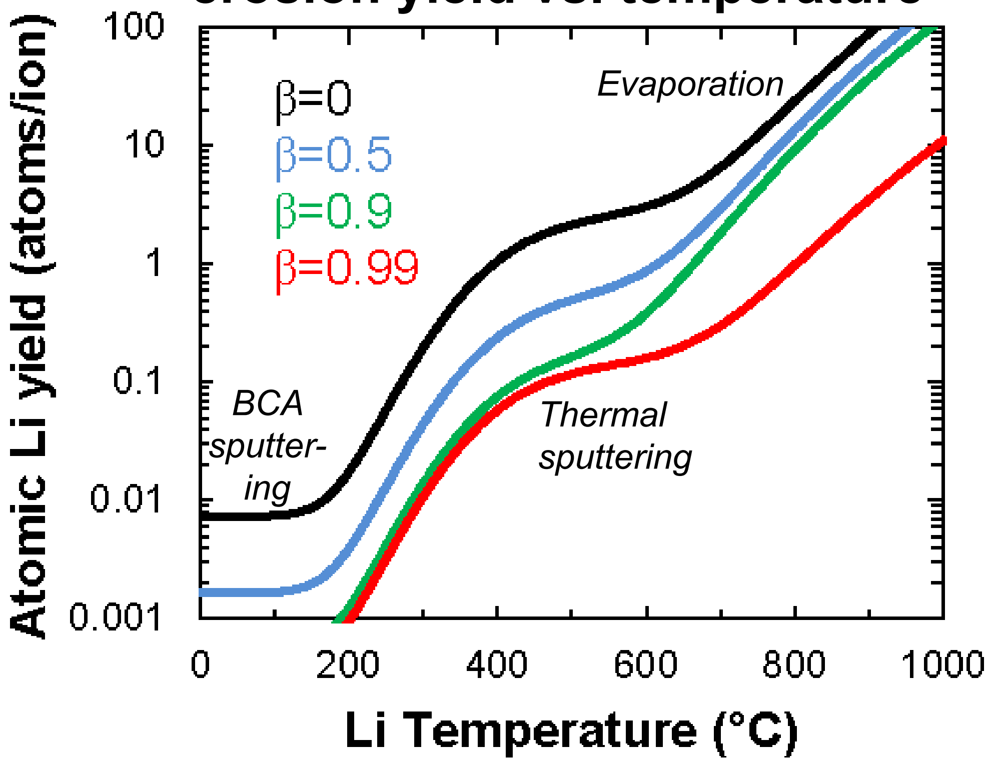
D/Li mixed-material reduction factor

2/3 of sputtered Li is Li+ (re-deposited)[a]

Thermally-enhanced sputtering (adatom-evaporation model)

Evaporation

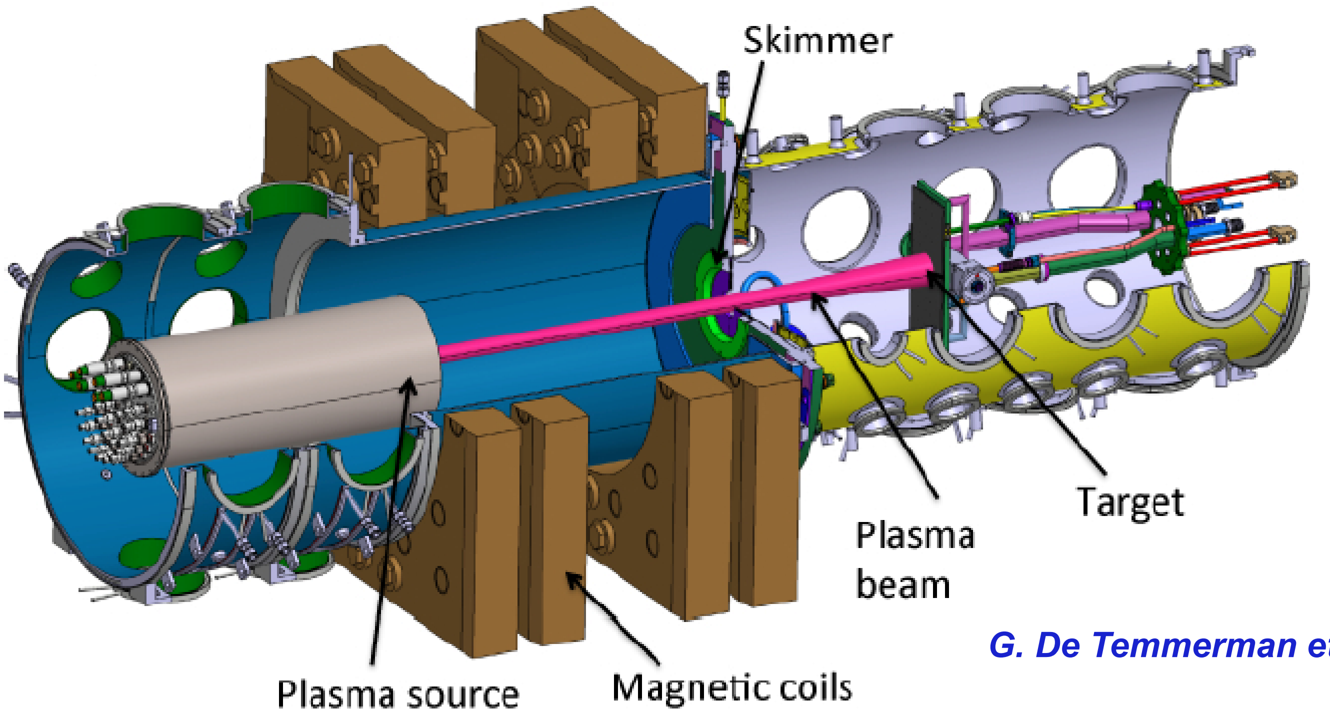
Mixed-material Li/LiD erosion yield vs. temperature



- Assume Y_{ad} and Y_{coll} are both reduced by ***f(β)***
  - Average of the **homogeous LiD** and **surface D monolayer** models
- Adatoms on a liquid?
  - Have been observed in MD simulations[b]
  - *A* is related to adatom lifetime τ
  - $\tau_{Li} >> \tau_{Be}$ (less vacancies on liquid)

[a] *K. Nordlund et al. Lett. Nat. 1999*
[b] *J.P. Allain et al., Phys. Rev. B 2007*

Model tested and analyzed in Magnum-PSI linear plasma device

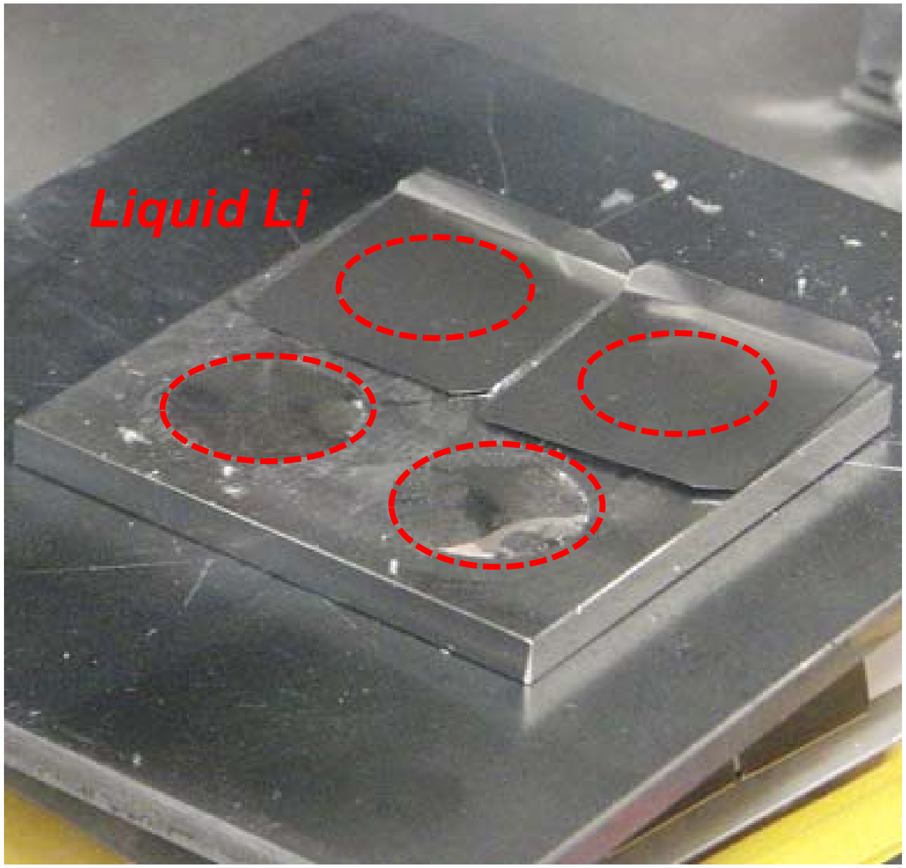


G. De Temmerman et al., FED 2013

- $\Gamma_{D+} \lesssim 2*10^{24}$ $m^{-2}s^{-1}$, $T_e \lesssim 3$ eV, $n_e \lesssim 8*10^{20}$ m^{-3}
- 5-10 s pulses, B = 0.25 T at target, 20-40 V bias
- Normal incidence: no magnetic pre-sheath
- Two sample types (both 2.5 cm diameter)
  - Evaporated Coatings (≤ 1 μm)
  - Shallow Li cups (0.1 – 1.0 mm)

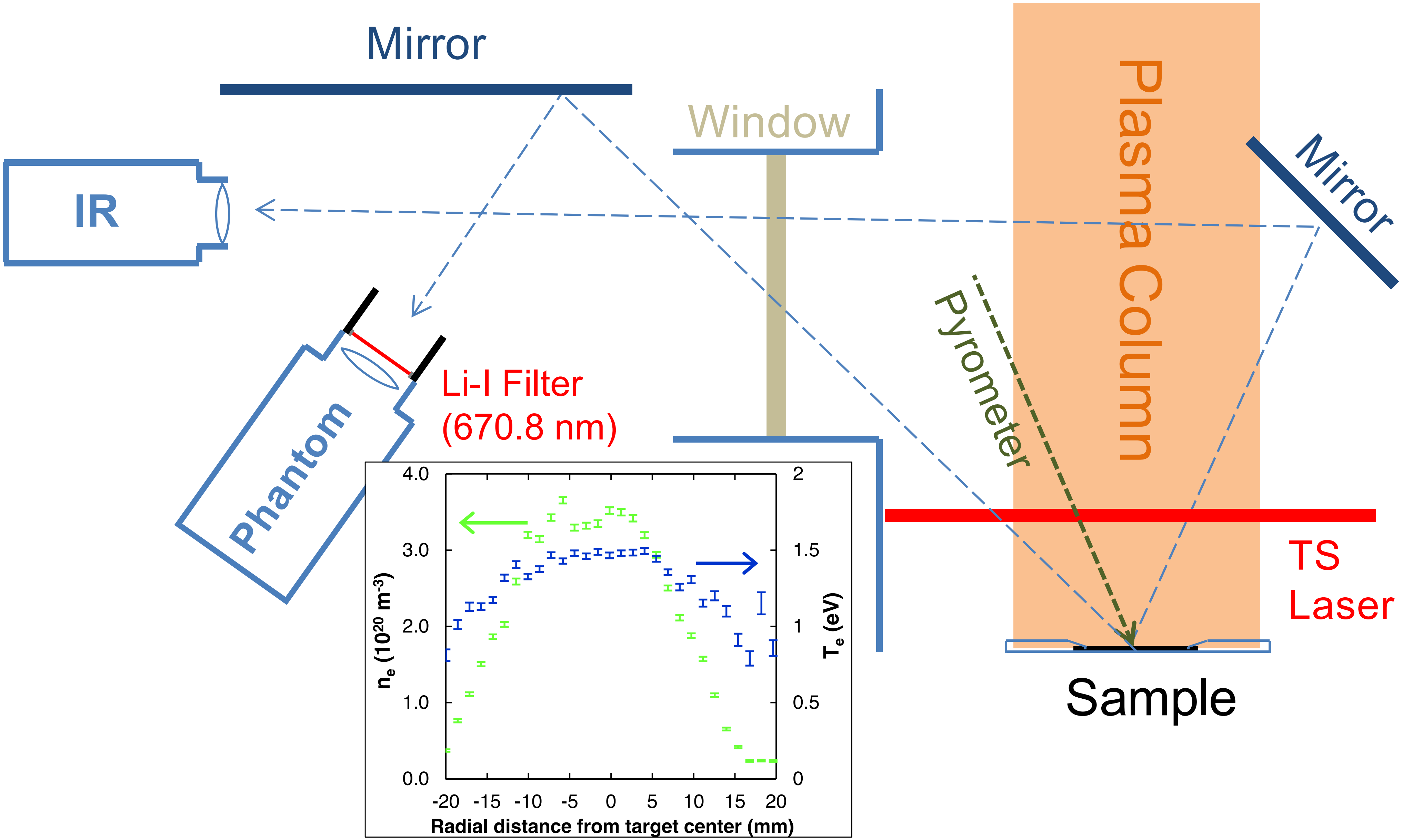
New procedure developed for loading 0.1-1.0 mm thick Li targets in Magnum-PSI sample holder

1. Li melted into sample wells inside Ar glove box
2. Sealed with SS shim stock covers & heat-seal mylar bags
3. SS cover remained on sample during mounting
4. Li exposed to atmosphere for 20-30 s between cover removal & vessel pumpdown
5. Ar plasma discharges used to remove oxide coating from Li



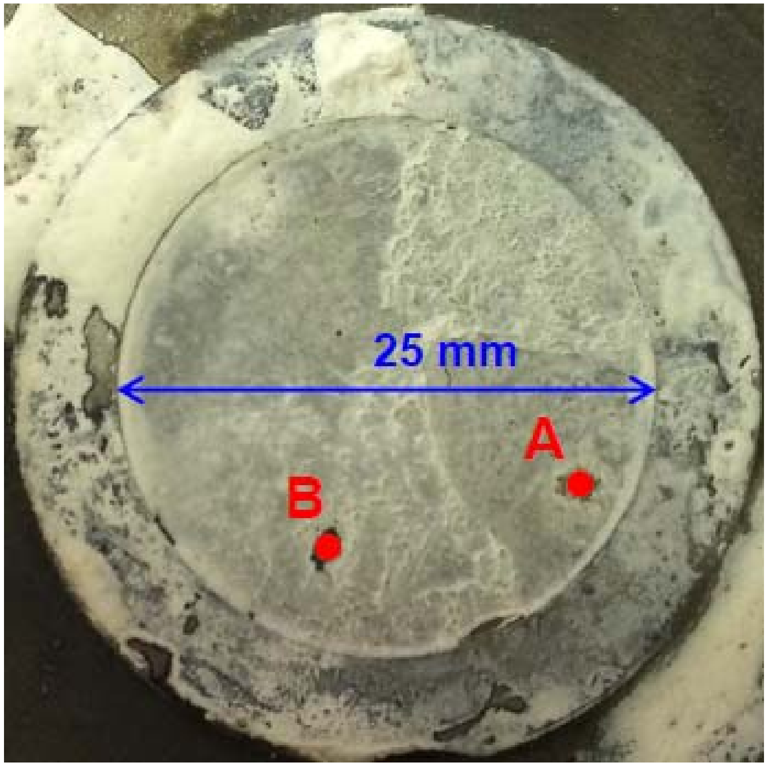
Four Li samples melted into wells on a SS prototype plate (two with shim stock covers)

Diagnostic suite provides measurements of plasma n_e/T_e, Li-I impurity radiation, and sample temperature



Macroscopic melt motion observed during Ar plasma cleaning of thick Li coatings

- Quickly reduces coating from its initial value of 500 μm
- Resulting thickness of Li coating measured for a sample exposed to a single Ne plasma shot
  - Measured via confocal microscopy
  - Assumed that coating expands along z direction only during conversion to Li carbonate
- Motivates modeling of β(t) for reduced Li thicknesses



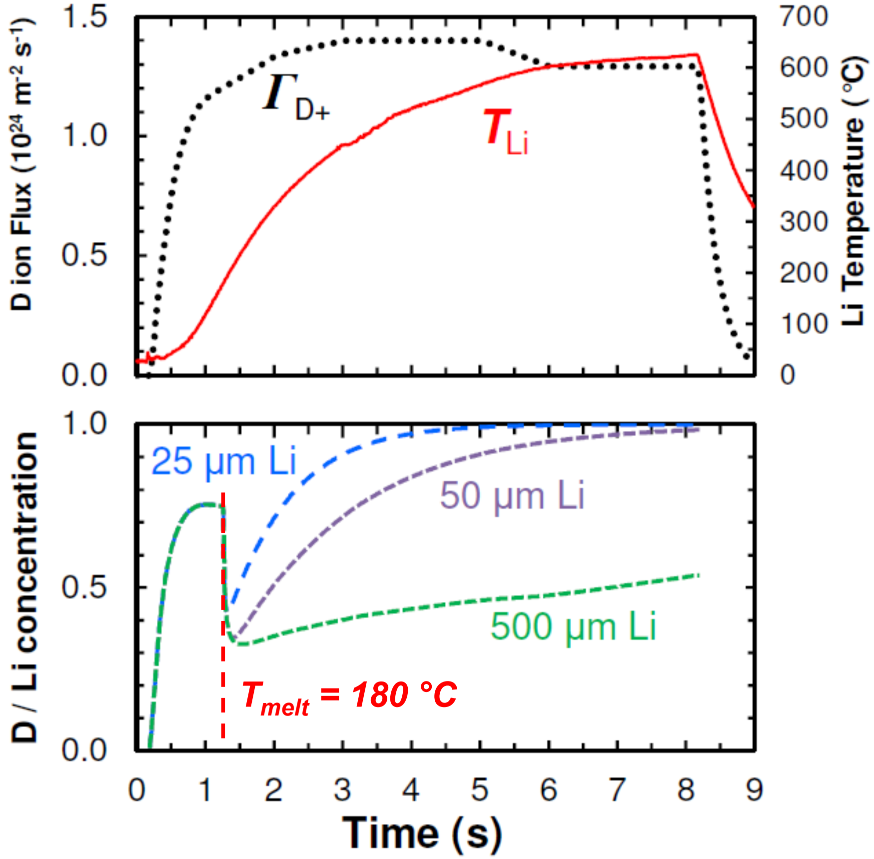
Position (mm)	Point A thickness (μm)	Point B thickness (μm)
0.5	25	56
1.0	30	167
1.5	39	125
2.0	40	132
2.5	7	156

Mixed-material Li erosion model can be tested by varying 1) ion species 2) total D fluence

1. Measure Li erosion rate during Ne plasma bombardment
   - Ne is not retained in or chemically reactive with Li
   - Thus model predicts no reduction in erosion rate at high fluxes

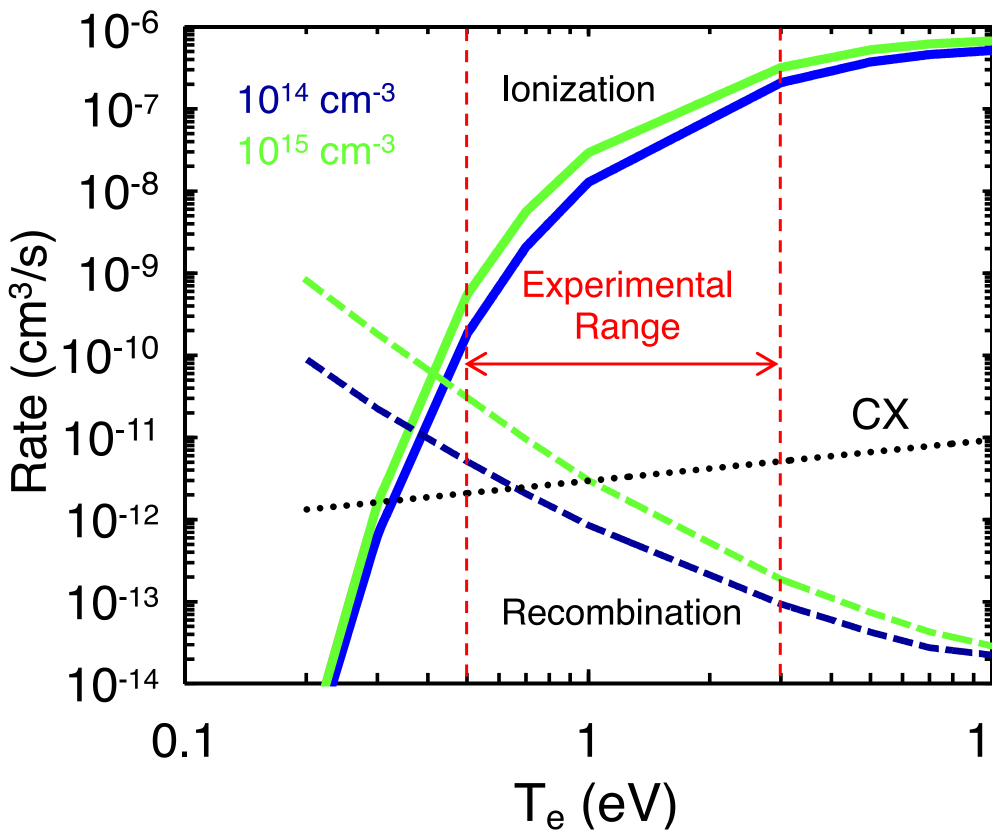
2. Measure Li erosion rate as β changes dynamically
   - $\beta(t)$ can be predicted using 1-D diffusion model for D in Li
   - Significant melt motion led to uncertainty in time evolution of Li thickness
   - Time evolution of β for various thicknesses were tested

Time Evolution of β, Γ_{D+}, and T_{Li} during typical Magnum-PSI discharge



Li-I emission rates can be interpreted using atomic data from ADAS collisional-radiative model*

Assumption	% Error
Collisional-radiative model	~0.1
Steady-state	$\sim 10^{-4}$
No recomb./CX	0.01 – 1
No ⊥ impurity transp.	0.5 – 5
No second. elect. emiss.	10^{-20}
No radiation trapping	1 – 10



$$\frac{\partial n_{\mathrm{Li0}}}{dt} + \nabla \cdot (n_{\mathrm{Li0}} v_{\mathrm{Li0}}) = -n_{\mathrm{Li0}} n_e S + n_{Li+} n_e R + n_{Li+} n_D C$$

*H.P. Summers, "Atomic Data and Analysis Structure User Manual," 2004. (www.adas.ac.uk)

Li yields inferred from Li-I emission measurements

- Solve Li^0 continuity equation with boundary condition:

v_{Li} = 5200 m/s (1 eV)

$$\nabla \cdot (n_{\mathrm{Li}} v_{\mathrm{Li}}) = -n_{\mathrm{Li}} n_e S_{Li}$$

$$n_{Li} v_{Li} \Big|_{z=0} = Y_{Li} \Gamma_{D+}$$

Ionization rate coefficient (ADAS)

- Solve for $n_{Li}(r, z, Y_{Li})$
- Model for Li-I photons / m^2 s:

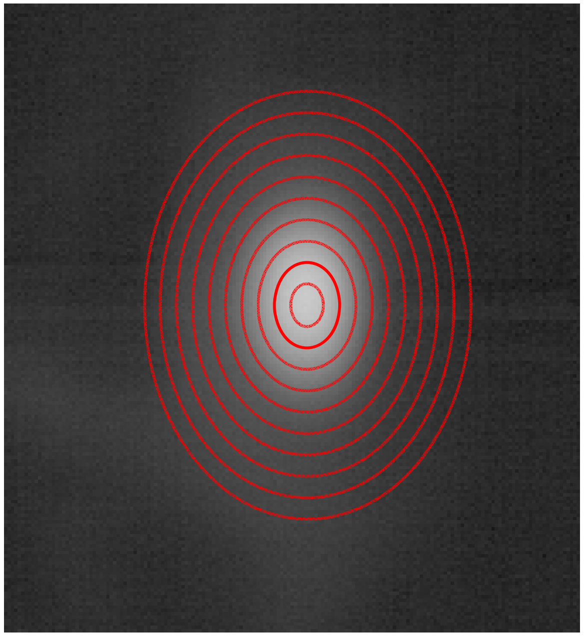
Photon emissivity coefficient (ADAS)

$$I_{Li,model} = \int_0^{z_0} n_{Li} n_e P_{Li}\, dz$$

- Axially averaged measurement:

$$I_{Li,meas} = T \frac{\Omega_{pixel}}{4\pi} \left(\frac{photons}{s} \right)_{meas}$$

- Set $I_{Li,model} = I_{Li,meas} \rightarrow$ **infer** Y_{Li}



Axially average Li-I emission

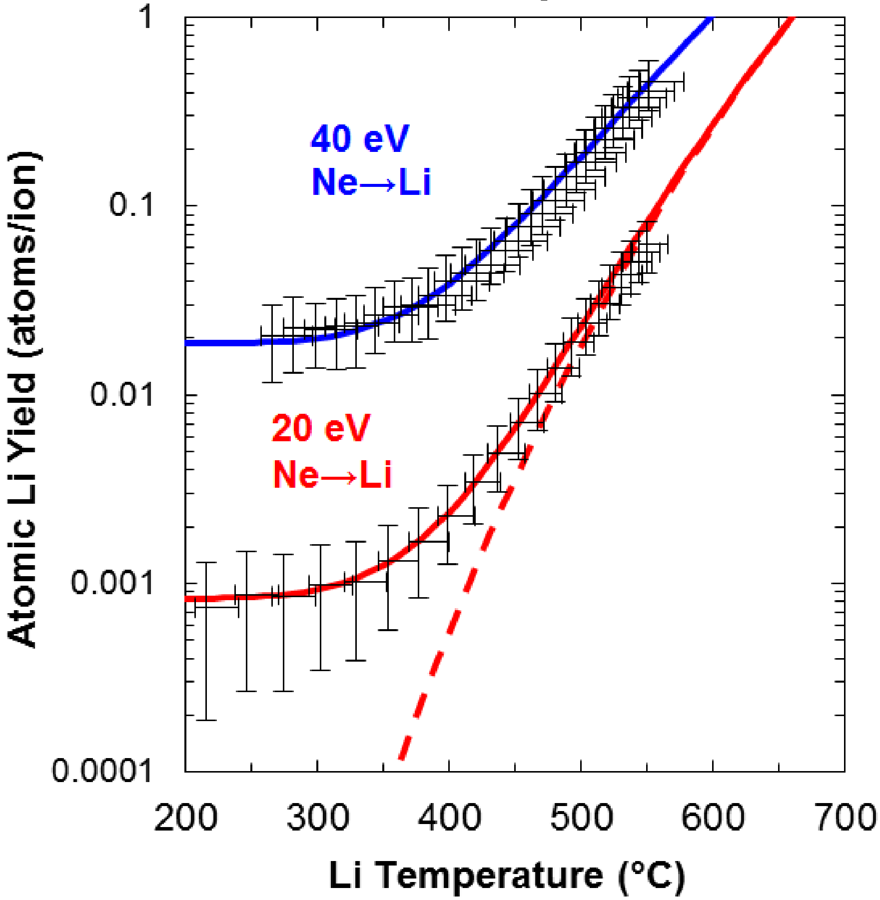
Li yields measured during Ne plasma bombardment are greater than Langmuir Law evaporation

- Suggests erosion model is valid for H-free Li films (β=0)

- 20 eV Ne→Li erosion much lower than 40 eV
  - Model predicts T-dependent sputtering is independent of E_{Ne+}
  - Possible near-threshold effects for Ne

- 40 eV Ne →Li consistent with previous results for He →Li

Atomic Li Yields Γ_{Li}/Γ_{Ne+} vs. Li Temperature

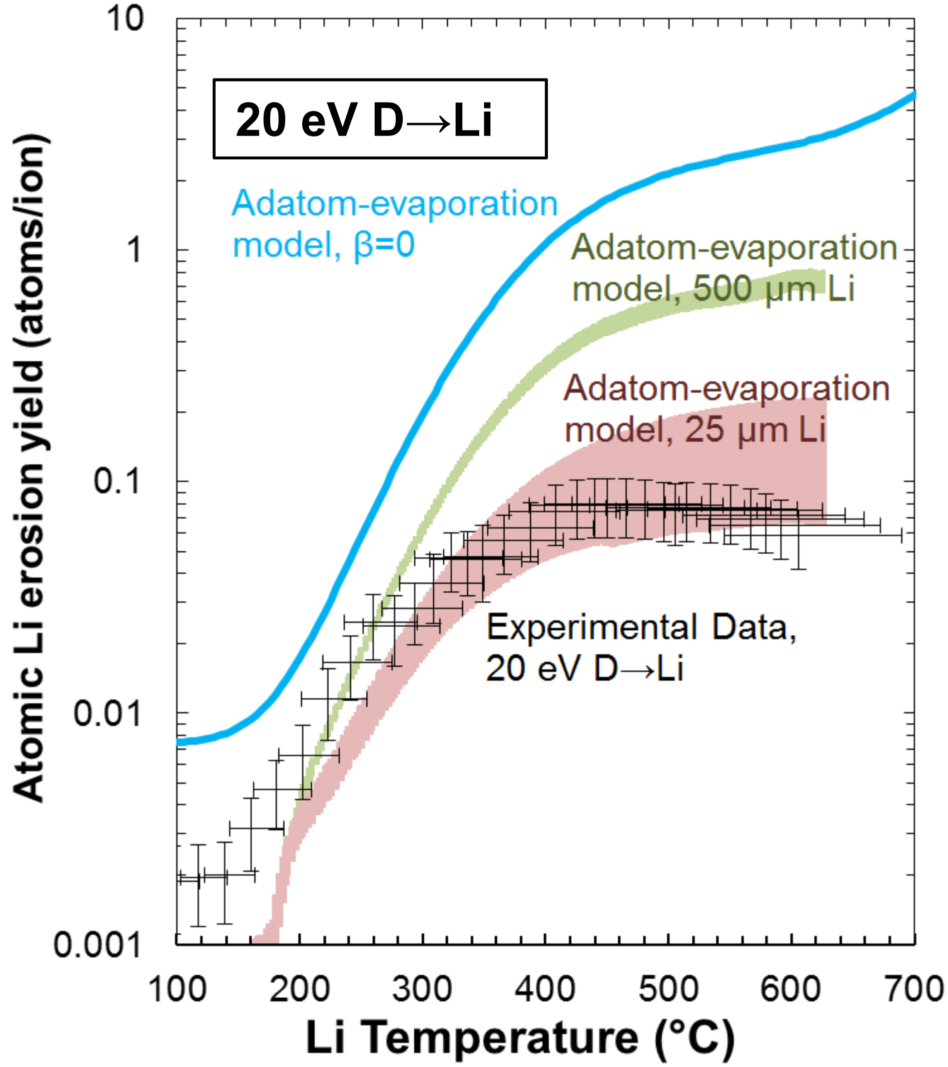


Solid line: Thermal-spike or adatom model (indistinguishable)
Dashed line: Evaporation only
Error bars: Experimental measurements

Li yields measured during D plasma bombardment compared to predictions of adatom mixed-material model

- Error band is distance between homogenous & partial D monolayer surface models
- Adatom mixed-material model captures quantitative evolution of Li erosion rate
- *A priori* assumption that Li thickness reduced to 25 μm

Atomic Li Yield Γ_{Li}/Γ_{D+} vs. Li Temperature



Numerous physics possibilities have been considered

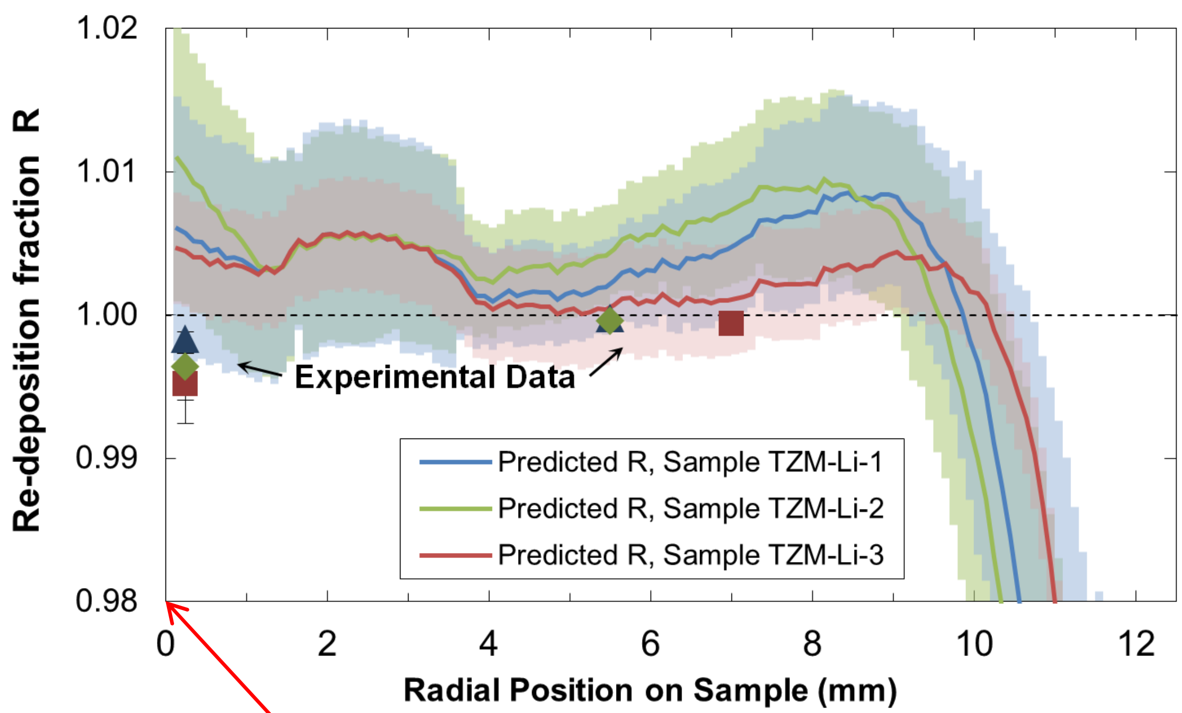
- Recomb./CX small, but would imply an even lower yield
- Γ_{D+} measured fairly constant 4.0-20 mm from target
- Drifts are almost entirely in azimuthal direction
- Results insensitive to v_{Li} (strong ionization)
- Transmission of optics measured before/after experiments
- Self-sputtering is small, would also imply even lower yield

Measured re-deposition fractions R for Li-coated TZM Mo are close to unity, as predicted by modeling

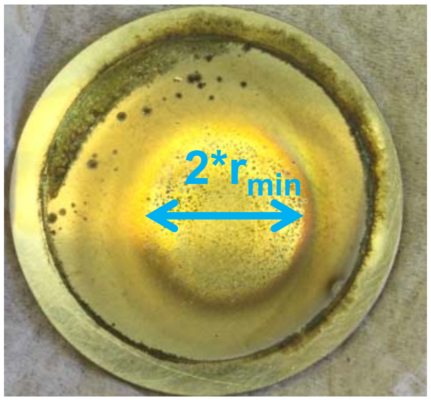
$$R = 1 - \frac{\rho_{\mathrm{Li}}}{\int_0^\tau Y_{\mathrm{Li}} \Gamma_{\mathrm{D+}} dt}$$

ρ_{Li} = Initial Li areal density

- At r=0: τ is the time when Li is depleted from sample center (Li-I emission ↓)
- A $r=r_{min:}$ τ is the full length of plasma discharges on sample



Note Suppressed Zero

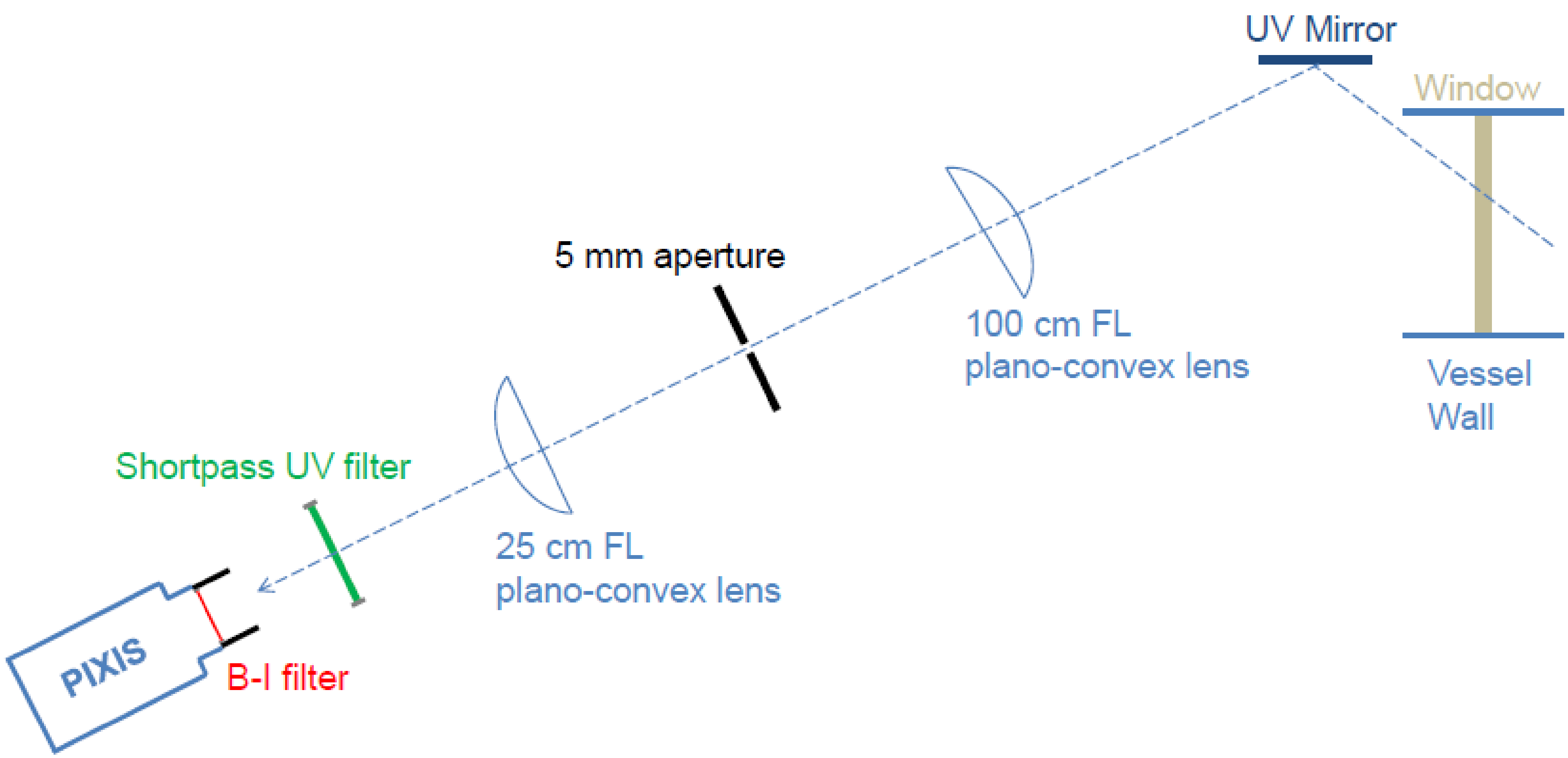


Photograph of Li sample immediately after removal from Magnum-PSI

Sample	$n_{e,peak}$	$T_{e,peak}$	Li Thickness	Duration
TZM-Li-1	$2.4*10^{20}$ m^{-3}	1.7 eV	190 nm	56 s
TZM-Li-2	$2.6*10^{20}$ m^{-3}	1.5 eV	190 nm	56 s
TZM-Li-3	$3.5*10^{20}$ m^{-3}	1.5 eV	190 nm	42 s

Preliminary measurements of boron erosion under high-flux D plasma bombardment have also been performed

- 300 nm B layers sputter-coated on TZM Mo
- No strong B lines in visible: use **249.7 nm** line
- Imaged with PIXIS 2040-B camera, ~4 Hz, 1 mm^2 res.
- Similar analysis applied to data using ADAS tables

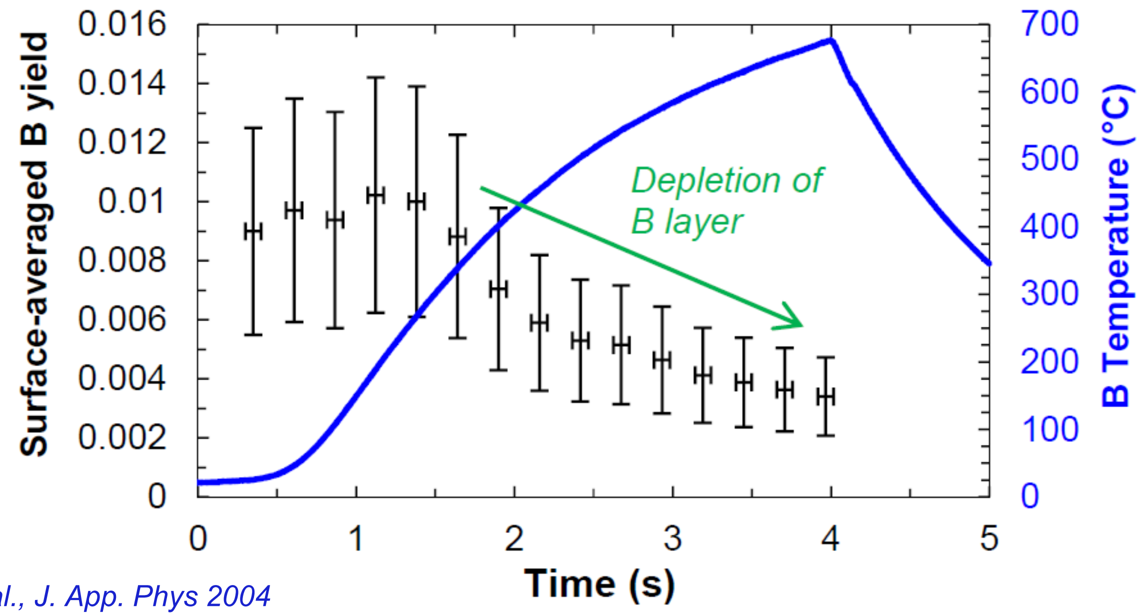


Preliminary measurements of boron erosion yield are significantly higher than on ion- beam experiments

- $\lambda_{iz,B} >> \lambda_{iz,Li}$
  - "Smearing" of erosion data
  - Can capture total B outflux w/o spatial resolution

- No T dependence, but not expected until $> 0.5*T_{melt}$[a,b] ($T_{melt,B}$ = **2076 °C**)

Surface-averaged B yield Γ_B/Γ_{D+} vs. B Temperature



[a]R.P. Doerner et al., J. App. Phys 2004
[b]H. Maier et al., PSI 2014

- Y_B >> previous measurement on ion beam device (0.004)
  - SBE of sputtered coating may be lower than bulk B
  - Conversion to boron oxide (B_2O_3) may have occurred
    - Yield could be enhanced via chemical sputtering
    - $Y_{B2O3} / Y_B \approx 15$ (TRIM.SP)

Predictions performed of how long a 100 µm Li coating will last under D plasma bombardment in NSTX-U divertor

- Series of 5 s pulses with thermal evolution:

$$T_{\mathrm{Mo}}(t) = T_0 + q\left(\frac{4\alpha_{\mathrm{Mo}}t}{\pi k_{\mathrm{Mo}}^2}\right)^{1/2}$$

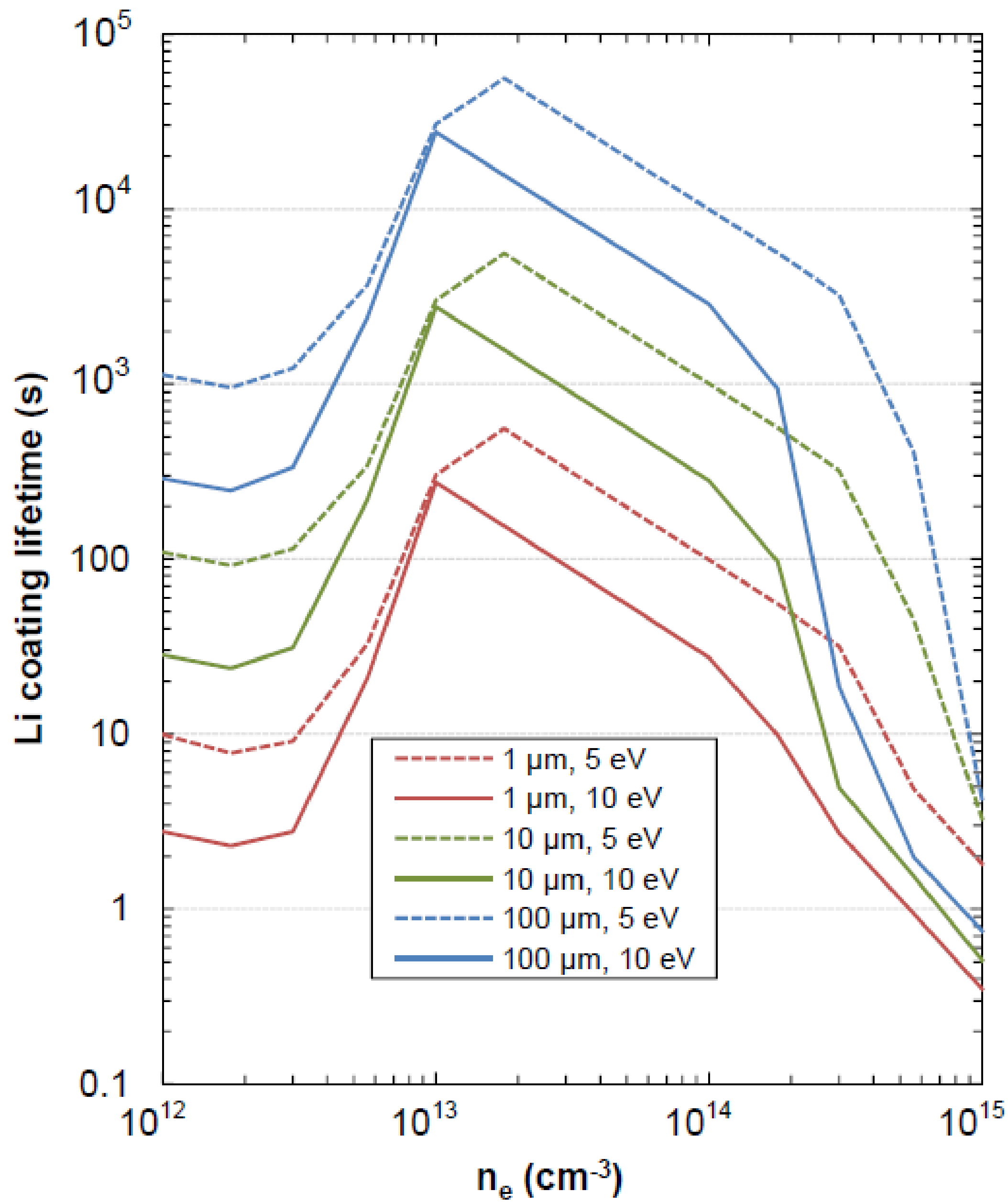
$$q = \frac{1}{2}\gamma n_e T_e c_s \sin\theta$$

$$\gamma = 8 \qquad \theta = 3^\circ$$

- Li lifetime calculated by solving for τ:

$$\int_0^\tau Y_{\mathrm{Li}}[T_{\mathrm{Li}}(t), \beta(t), \Gamma_{\mathrm{D+}}]\,dt = \frac{\rho_{\mathrm{Li}}}{(1-R)\Gamma_{\mathrm{D+}}}$$

- Note: R calculations are for linear plasma; R_{max} is specified as 0.99



Conclusions

- Adatom-evaporation mixed-material model developed to predict temperature-dependent Li+D erosion rates
- Techniques for inferring time and spatially dependent erosion yields developed using ADAS atomic phys. data
- Erosion yields of Li and B coatings on TZM Mo measured during high-flux bombardment on Magnum-PSI
- Model captures quantitative dependence of Li erosion yield for thick mixed-material Li/D layers
- B erosion measurements using B-I emission performed for the first time using custom-built optics system