NSTX-U

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NSTX-U Collaboration Research Plans for Princeton University Surface Science

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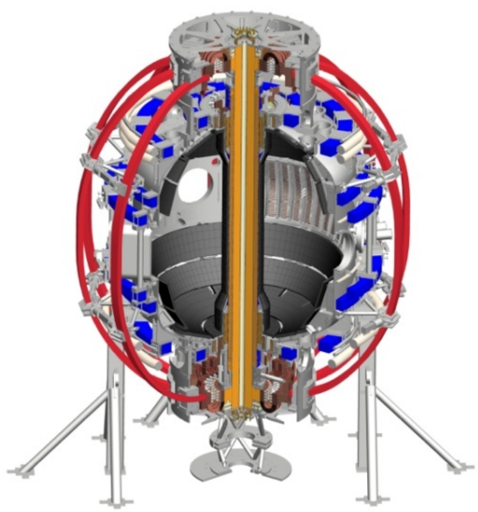
X Science LLC

Prof. Bruce E. Koel

Dr. J. Roszell, T. Thiem, with C.H. Skinner (PPPL)

and the NSTX Research Team

NSTX-U Physics Meeting, PPPL
March 18, 2015



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Fundamental surface science of PFCs for improved plasma performance in NSTX-U

Goal

Improve understanding of plasma surface interactions and specific information needed for NSTX-U operations and the future development of Li-conditioned plasma-facing components in high-heat flux long-pulse scenarios.

Approach

Quantitative measurements under controlled laboratory UHV conditions using surface sensitive probes including low energy ion scattering (LEIS) and high-resolution X-ray photoelectron spectroscopy (HRXPS) to characterize Li and complex mixed-material deposits on refractory metal single crystals (initially Mo) and practical alloys.

Surface chemistry and temperature dependence of surface properties such as D uptake and retention will be probed by temperature programmed desorption (TPD) mass spectrometry and vibrational spectroscopy using infrared spectroscopy (IR) and high resolution electron energy loss spectroscopy (HREELS).

Surface science of plasma-facing components

Plans

(i) D uptake and retention in mixed Li/C deposits on metal (*e.g.* Mo) PFCs, characterizing dependence on substrate temperature and impurities (*e.g.* O)

(ii) D interactions with mixed Li/O/B/C deposits on metal PFCs

(iii) quartz crystal microbalance (QCM) measurements to determine the temperature dependence of diffusion of O into bulk Li and strategies for removing contamination from Li surfaces

(iv) Li wetting experiments on TZM alloy and 316 stainless steel

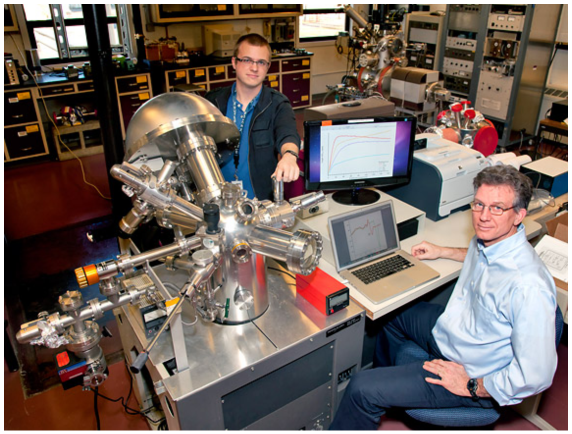
(v) composition and surface chemistry of Sn and Sn-Li alloys for longer-term PFC solutions, specifically the interactions of D atoms and ions with Li

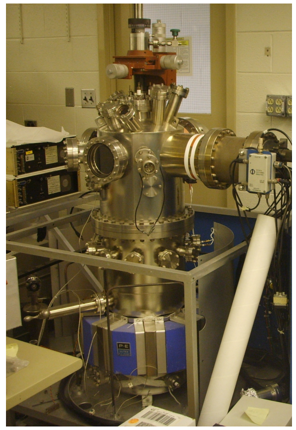
Deliverables

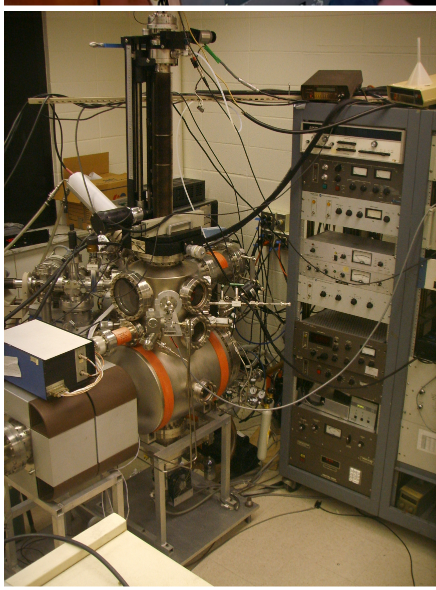
- Retention of D in Li and Li-C films versus temperature
- Retention of D in Li, Li-C, and Li/B/C films versus concentration of O
- Diffusion coefficient of O in solid and liquid Li; evaluation of possible reactive gases for removal of passivated Li films
- Surface diffusion coefficient of Li on various substrates
- D retention in Sn and Sn-Li films versus temperature and alloy composition

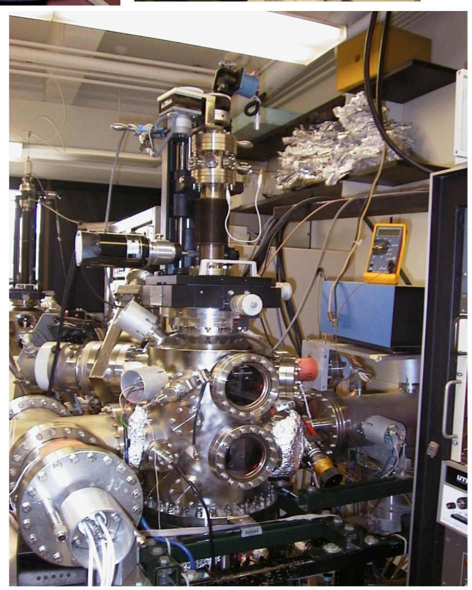
Materials characterization labs at PPPL

Surface Science and Technology Laboratory (SSTL)









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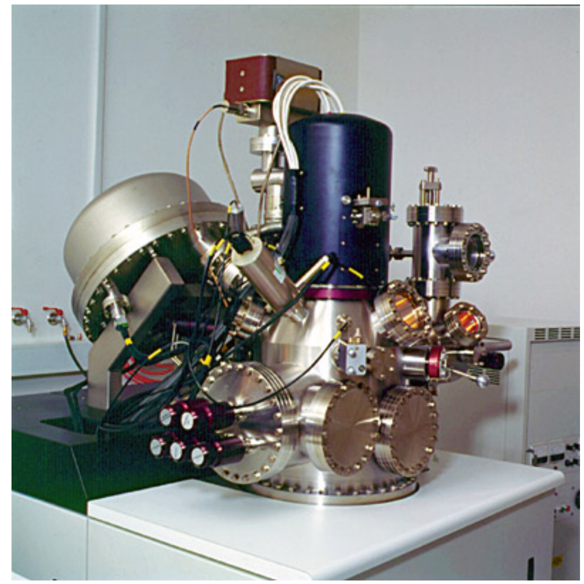
Surface Imaging and Microanalysis Laboratory (SIML)



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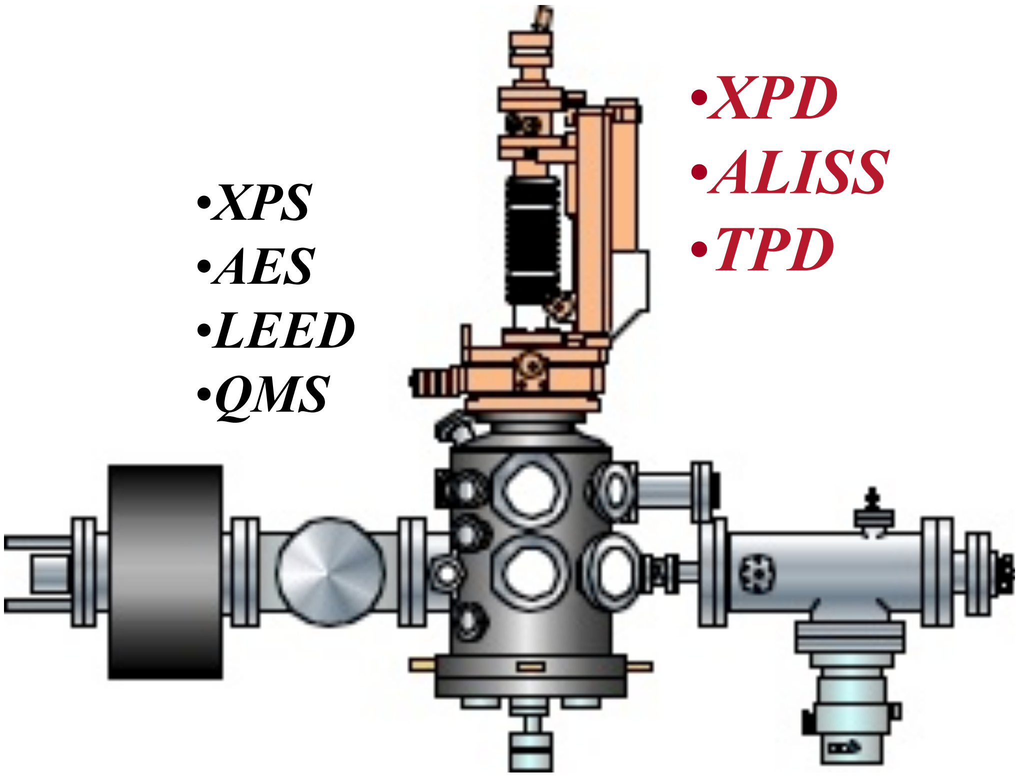
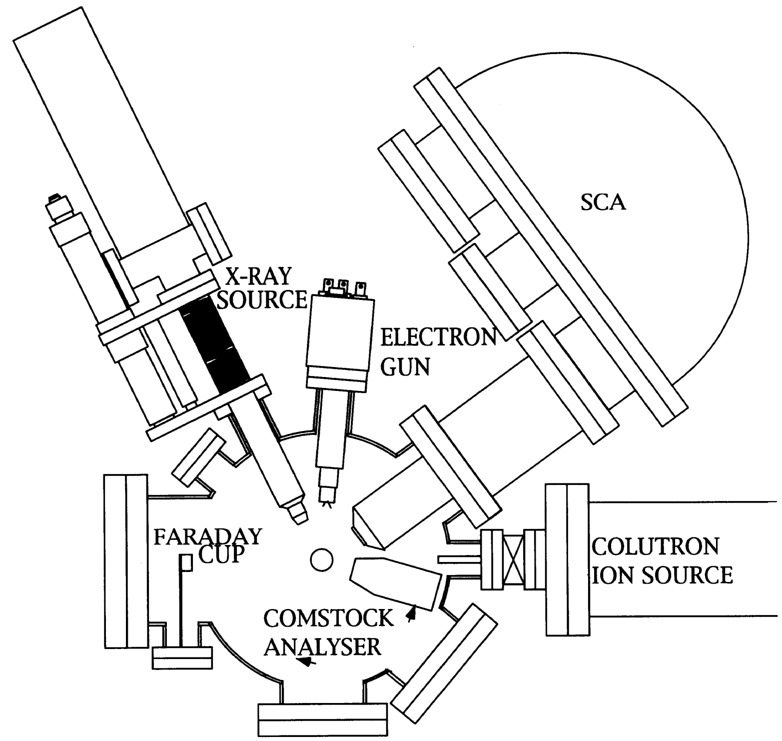
AES, XPS, XPD, UPS, HREELS, ELS, ESD, Δφ, LEED, RHEED, TPD, LEIS, ALISS, SAM, SEM

XPS/XPD/LEIS/ALISS instrument

- *XPS*
- *AES*
- *LEED*
- *QMS*



- *XPD*
- *ALISS*
- *TPD*

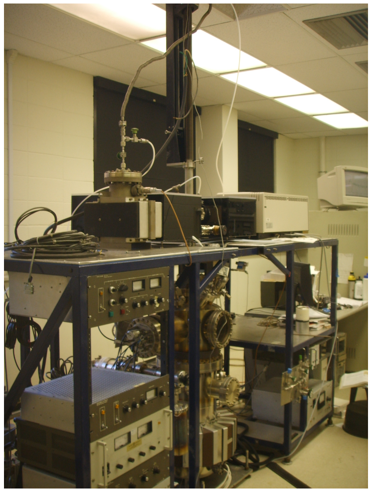


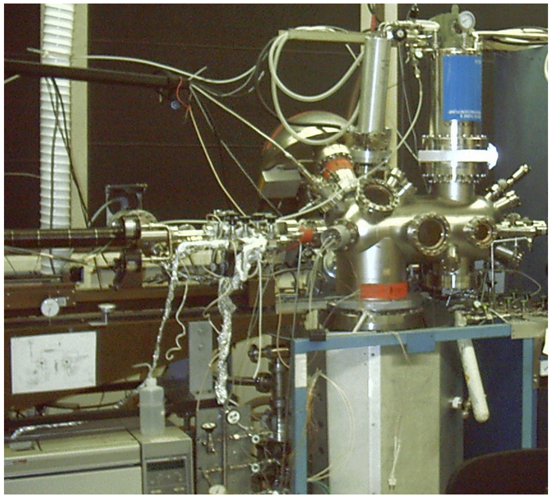
- ***Li deposition***
  Resistive heating of Li in crucible or SAES getter source

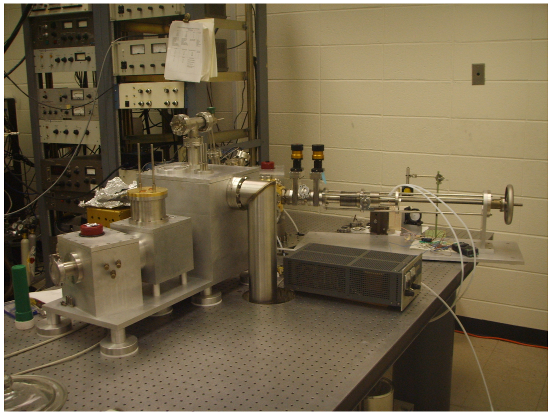
- ***Li film growth***
  Deposition of submonolayer or thicker Li films in vacuum or reactive gas environments and heat substrate to high temperature

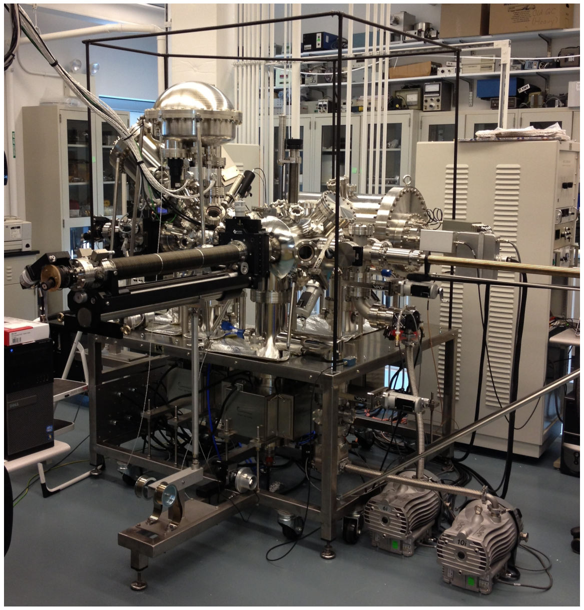
Surface science labs at PU

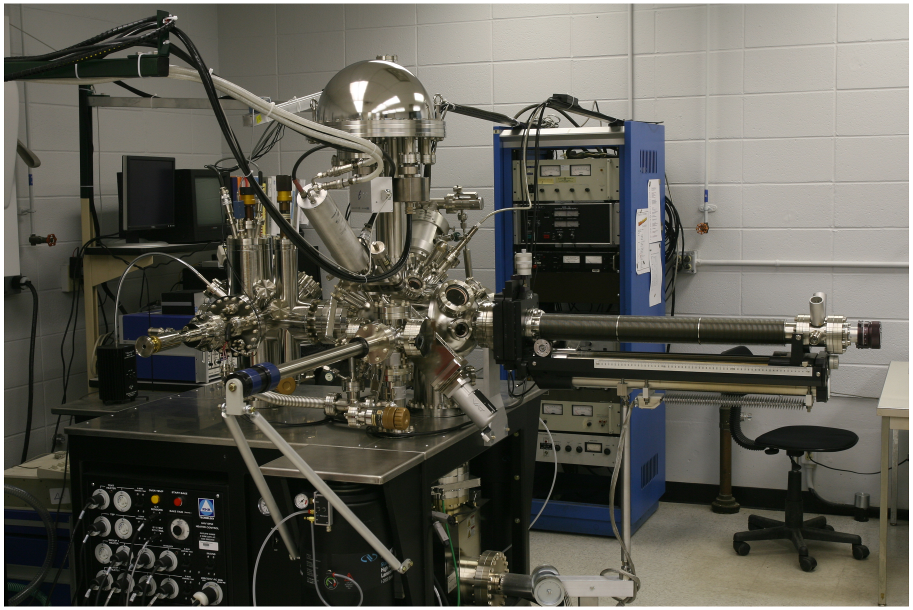
Laboratory for Surface Chemistry (LSC)











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Timetable of PU surface science activities

Year 1: Sept 2014 - Aug 2015

- Synthesize and characterize Li-C deposits *(Surface Science and Technology Laboratory (SSTL))*
- Migration of impurities through solid and liquid Li films *(SSTL)*
- Elementary rates of adsorption, scattering, and recombination for interactions of D_2, D atoms, and D^+ ions with Li-C deposits *(SSTL)*
- *High resolution electron and ion spectroscopy (HR-XPS, LEIS, RBS) to elucidate surface chemistry of Li/ B MAPP samples (Laboratory for Surface Chemistry (LSC))*
- *Collaboration to operate MAPP (Coordinate with JP Allain)*

Year 2: Sept 2015 - Aug 2016

- Temperature dependence of D uptake and retention in mixed Li-C deposits *(SSTL)*
- Compare experimental results to quantum-classical MD calculations by P. Krstić
- Synthesis and characterization of Li/O/B/C deposits *(SSTL)*
- Li wetting on TZM and stainless steel using Scanning Auger Microprobe (SAM) *(Surface Imaging and Microanalysis Laboratory (SIML))*
- Bulk oxidation of lithium layers *(SULI project 2014)*
- *Surface spectroscopy to complement MAPP analysis*

Timetable of PU surface science activities

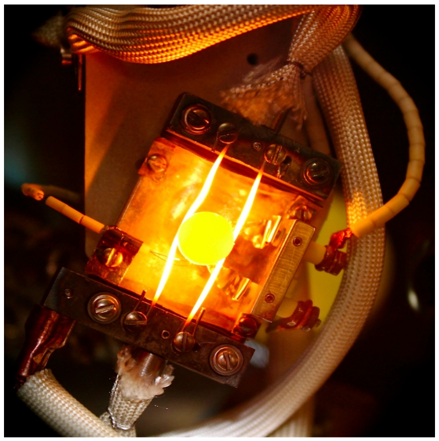
Year 3: Sept 2016 - Aug 2017

- Temperature dependence of D uptake and retention in Li/O/B/C deposits *(SSTL, some preliminary results already)*
- Removal of oxidized lithium layers by reactive gases *(SSTL)*
- Li wetting on TZM and stainless steel *(SIML, some preliminary results already)*
- *Surface spectroscopy to complement MAPP analysis*

Year 4: Sept 2017 - Aug 2018

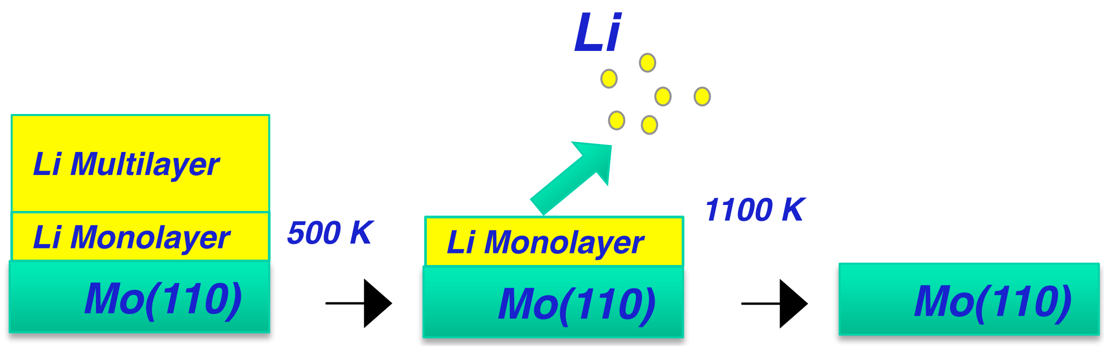
- Expand characterization and surface chemistry studies to more complex mixed deposits *(SSTL)*
- Effect of D, O, and C on wetting and adhesion of Li *(SIML)*
- Surface science studies of Sn and Sn-Li alloys *(SSTL)*
- *Surface spectroscopy to complement MAPP analysis*

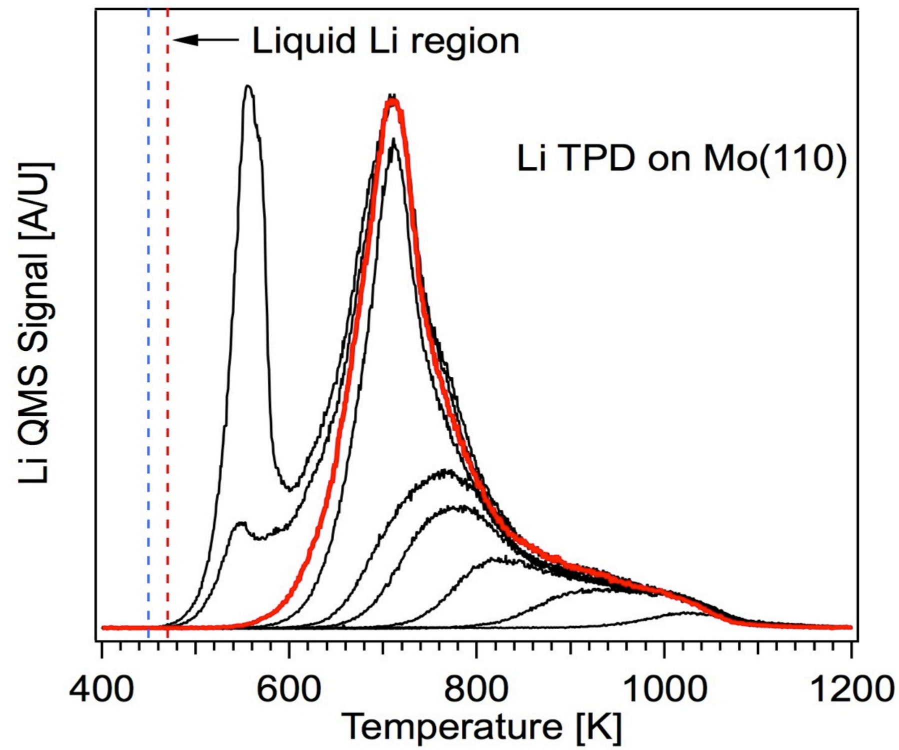
Thermal stability of Li on Mo(110)



Mo(110) resistively heated in UHV

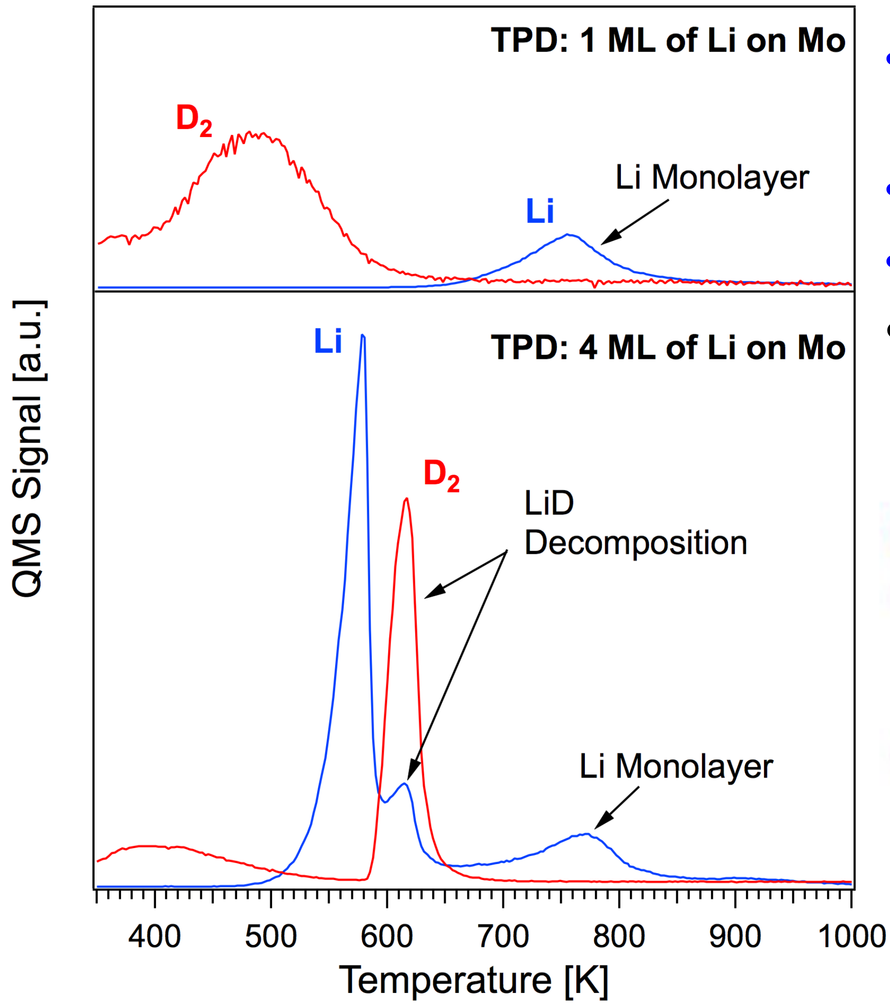
- Area under TPD curve is proportional to atoms desorbed
- Red curve is 1 ML Li; 0.5 nm thick
- Sub-monolayer control of film thickness
- Liquid Li films are stable between 450-470 K
- Desorption peaks correlated with binding (adsorption) energies



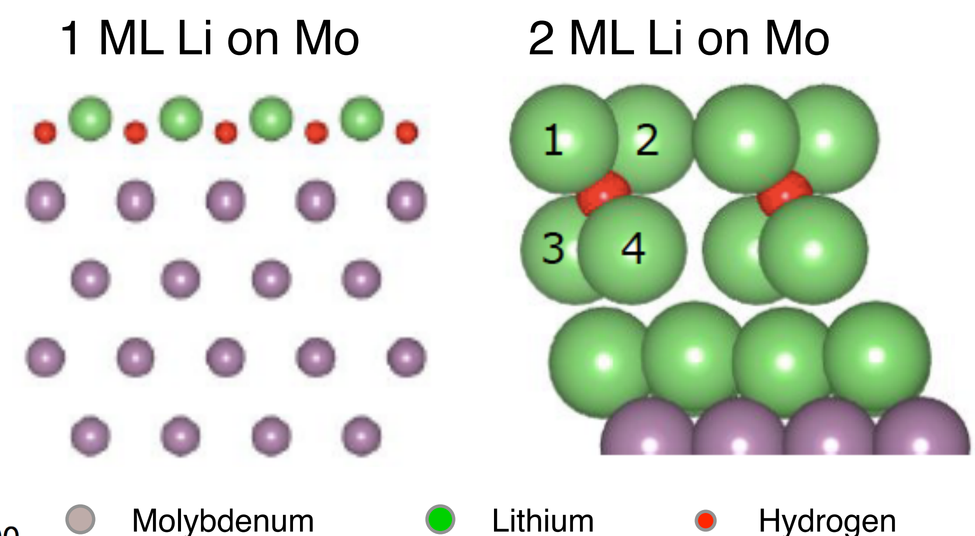


D retained as LiD in Li multilayer films

Li-Mo bonding stronger than Li-D

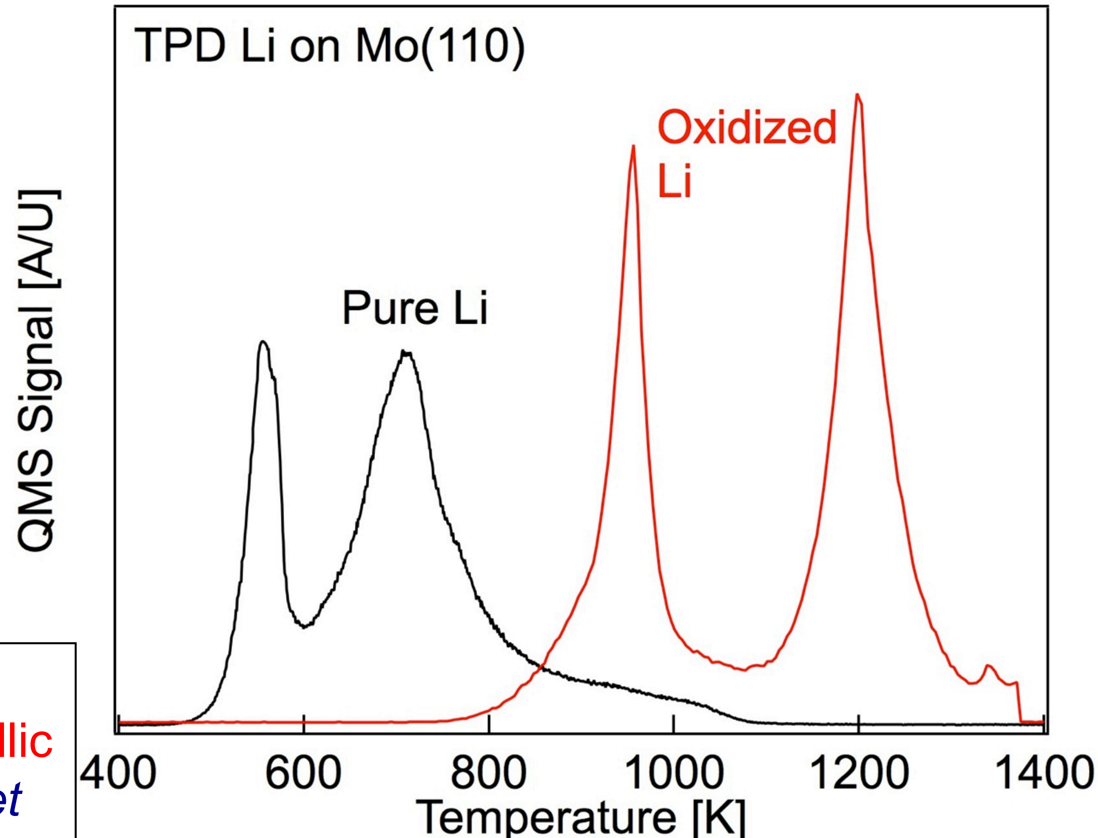


- DFT calculations show implanted D binds with Mo when 1 ML Li present
- With 2 ML, Li_4D complexes predicted to form
- (DFT by Chen, Carter, Princeton U.,
- DOE FES *"Atoms to Tokamaks"* grant



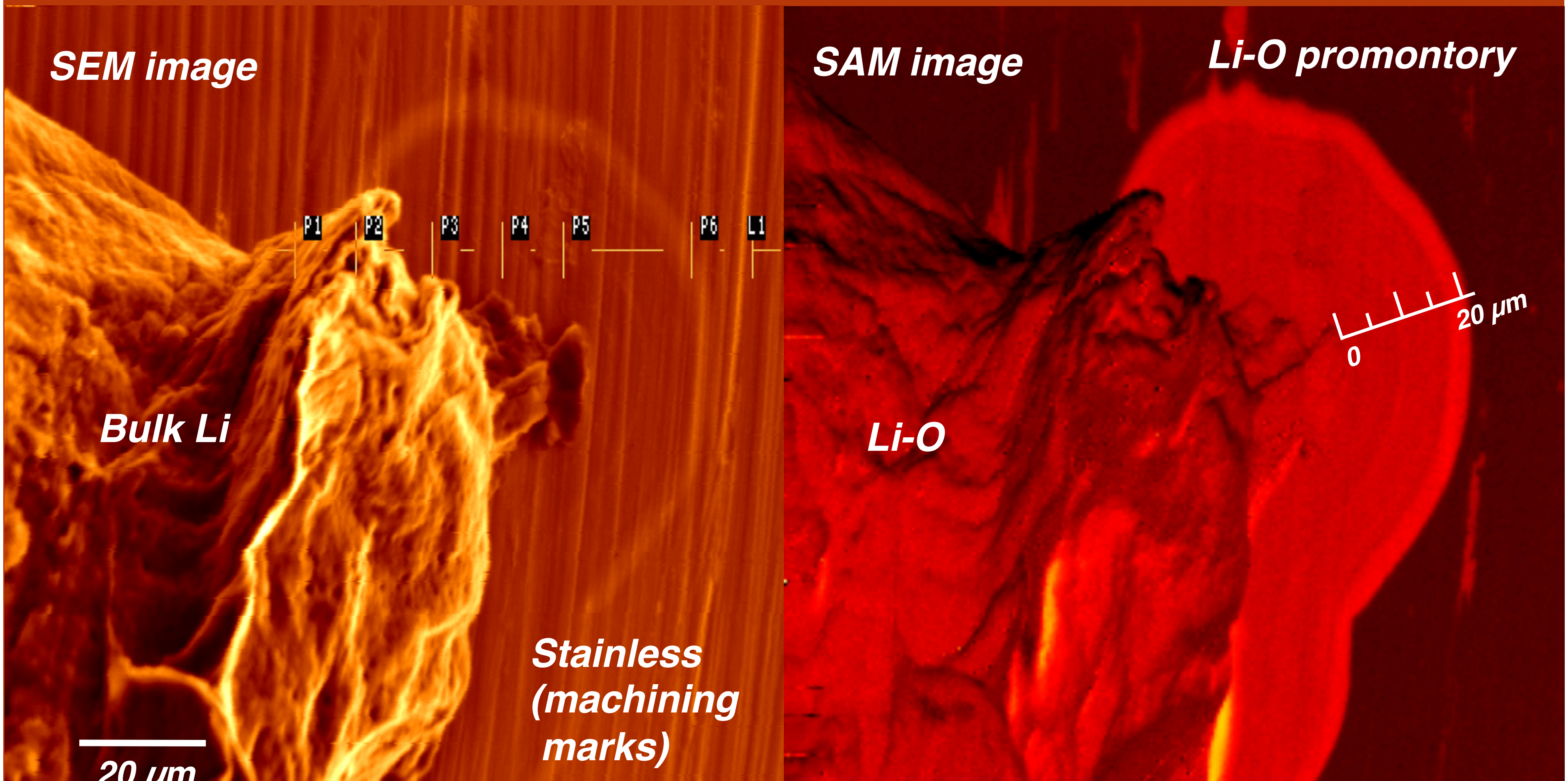
Lithium oxides are stable up to high temperature

- Oxidized Li has different chemical and thermal stability than pure Li
- Lithium oxides are stable up to 900 K
- Li-containing film stability is increased by 400 K (500 → 900 K)



- Tokamak plasmas initially see Li oxide walls rather than pure metallic Li (*Sullenberger thesis; Skinner et al, JNM 438 (2013) S647)*
- Important to measure D retention and erosion rates on Li_2O

Surface diffusion of Li on stainless steel + 14d

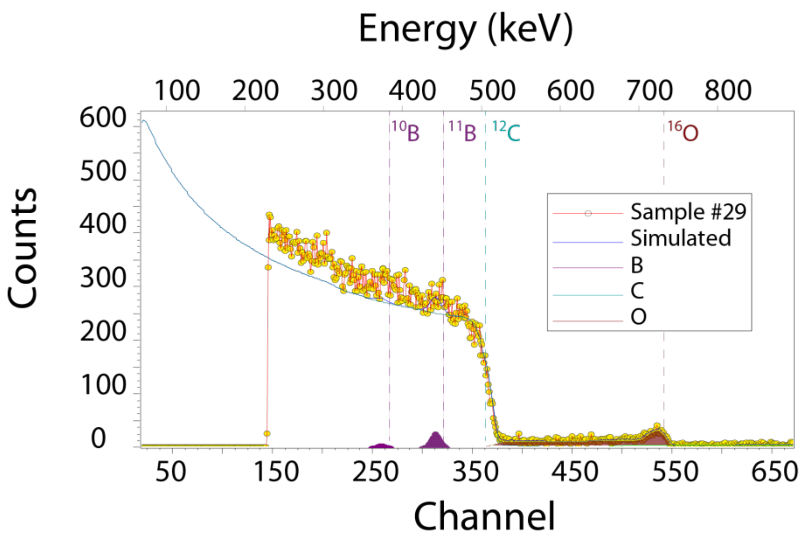


SEM image **SAM image of Li-O**

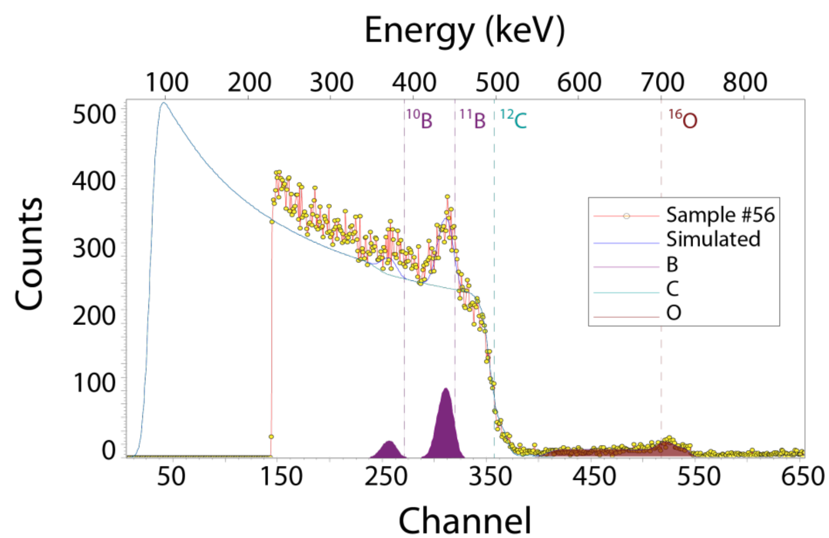
14 days after Ar etching (surface Li oxidized)

RBS: ~5x higher B bulk concentration for type II

Type I boronization



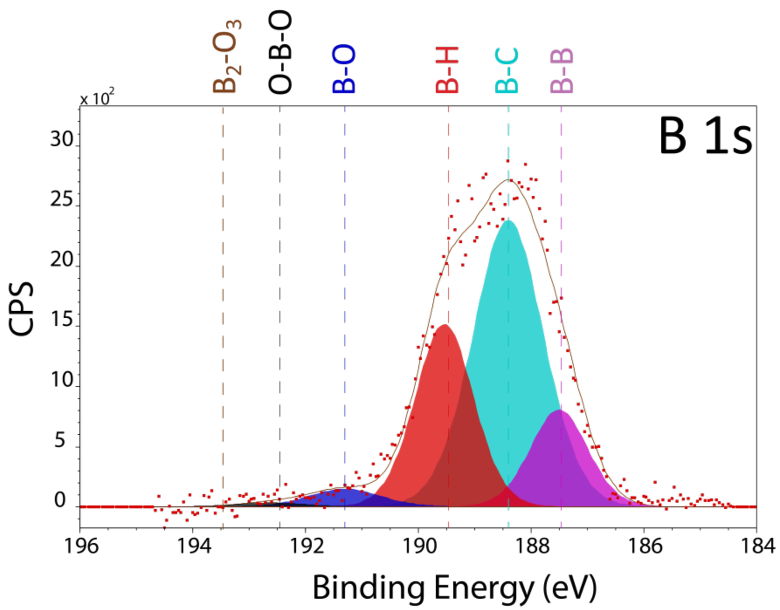
Type II boronization



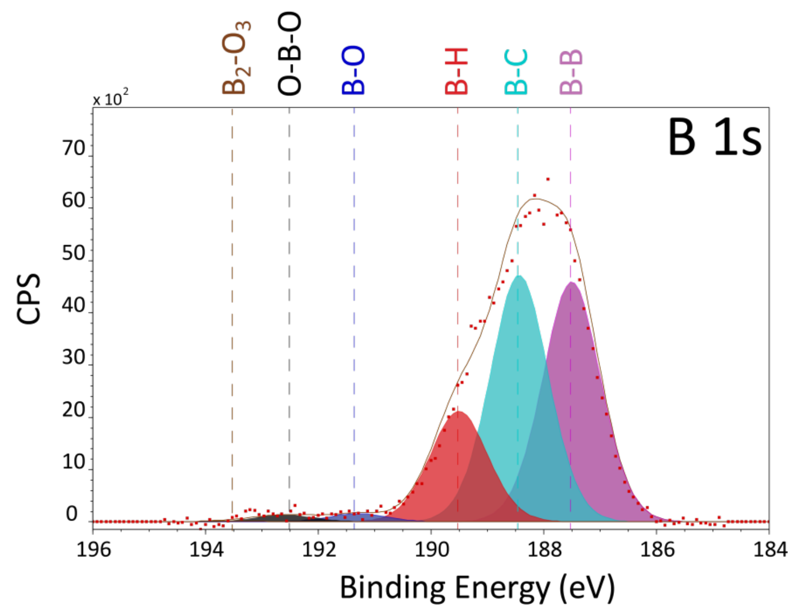
	Peak area	
	Type I (#29)	Type II (56)
Boron	0.74%	3.55%
Carbon	98.20%	95.53%
Oxygen	1.06%	0.92%

HRXPS: surface chemical composition - B1s line

Type I boronization



Type II boronization



	Position (eV)	FWHM (eV)
B-B	187.5	1.162
B-C	188.4	1.5
B-H	189.5	1.1
B-O	191.3	1.5
O-B-O	192.6	1.5
B_2-O_3	193.5	1.5

Plans for 2015 run

- Use HR-XPS and other spectroscopies to elucidate chemistry of lithiated and boronized samples

  Do beneficial Li / B effects correlate with Li / B surface composition?

- Use samples exposed by MAPP; transport samples to SSTL, SIML, and LSC in Ar atmosphere
- Initially day-long exposures. Correlate with individual discharge conditions when MAPP probe drive is automated
- Piggyback on runs for other XPs for the most part
- Low triangularity discharges preferred to increase flux on MAPP samples
- Detailed analysis of coupons and tiles retrieved at end of campaigns