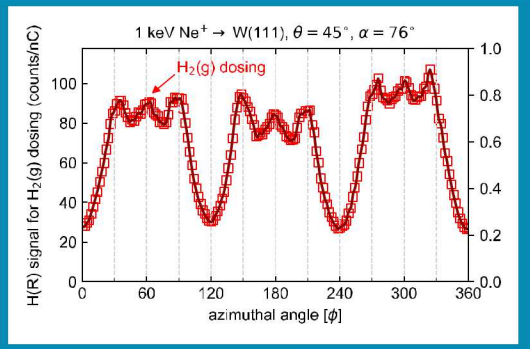
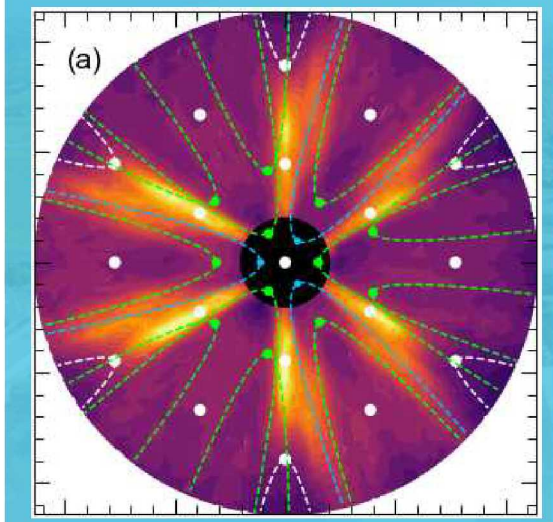
SAND2019-14041C

Characterization of W(111)+H(ads) system using multi-angle scattering and direct recoil maps





PRESENTED BY

Chun-Shang "Tim" Wong | November 18, 2019

Robert Kolasinski and Josh Whaley

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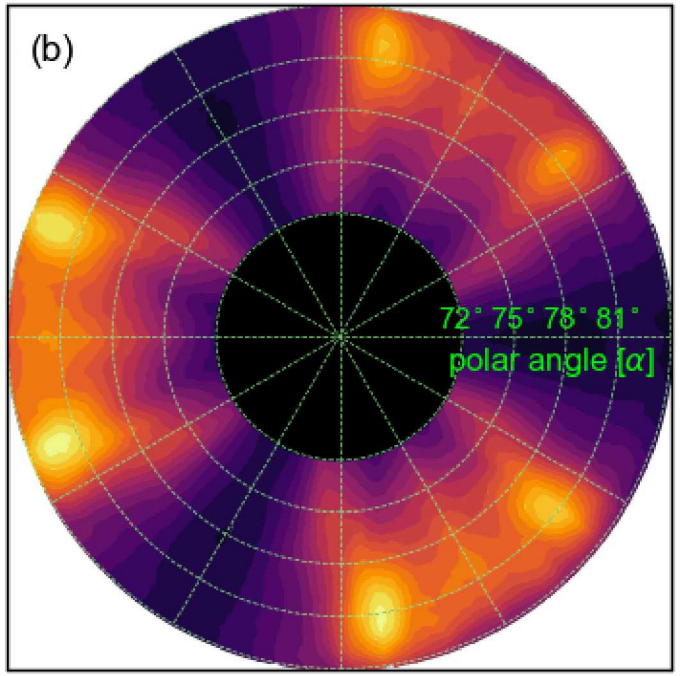
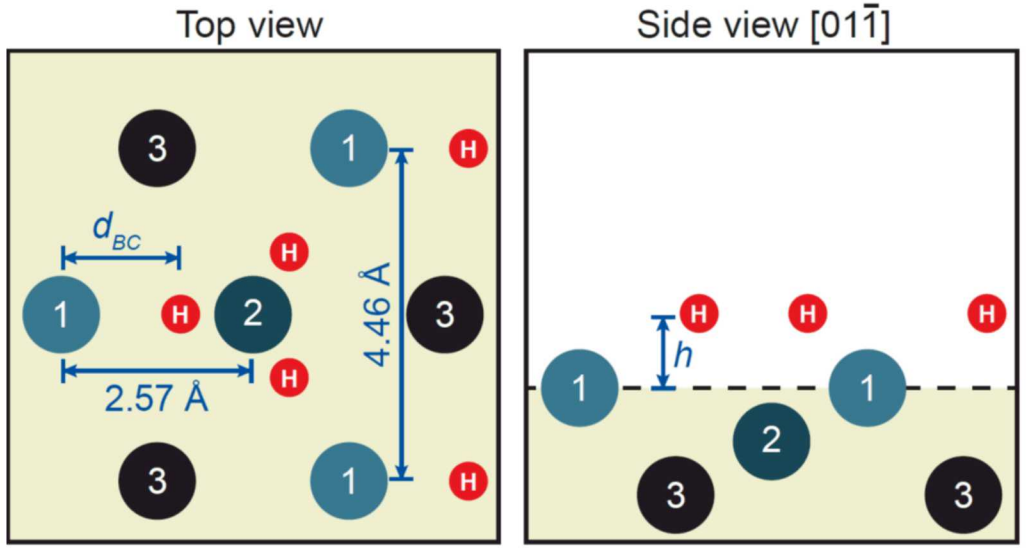
Outline

- Hydrogen interactions with tungsten surfaces
- Characterizing the W(111)+H(ads) system
- Summary

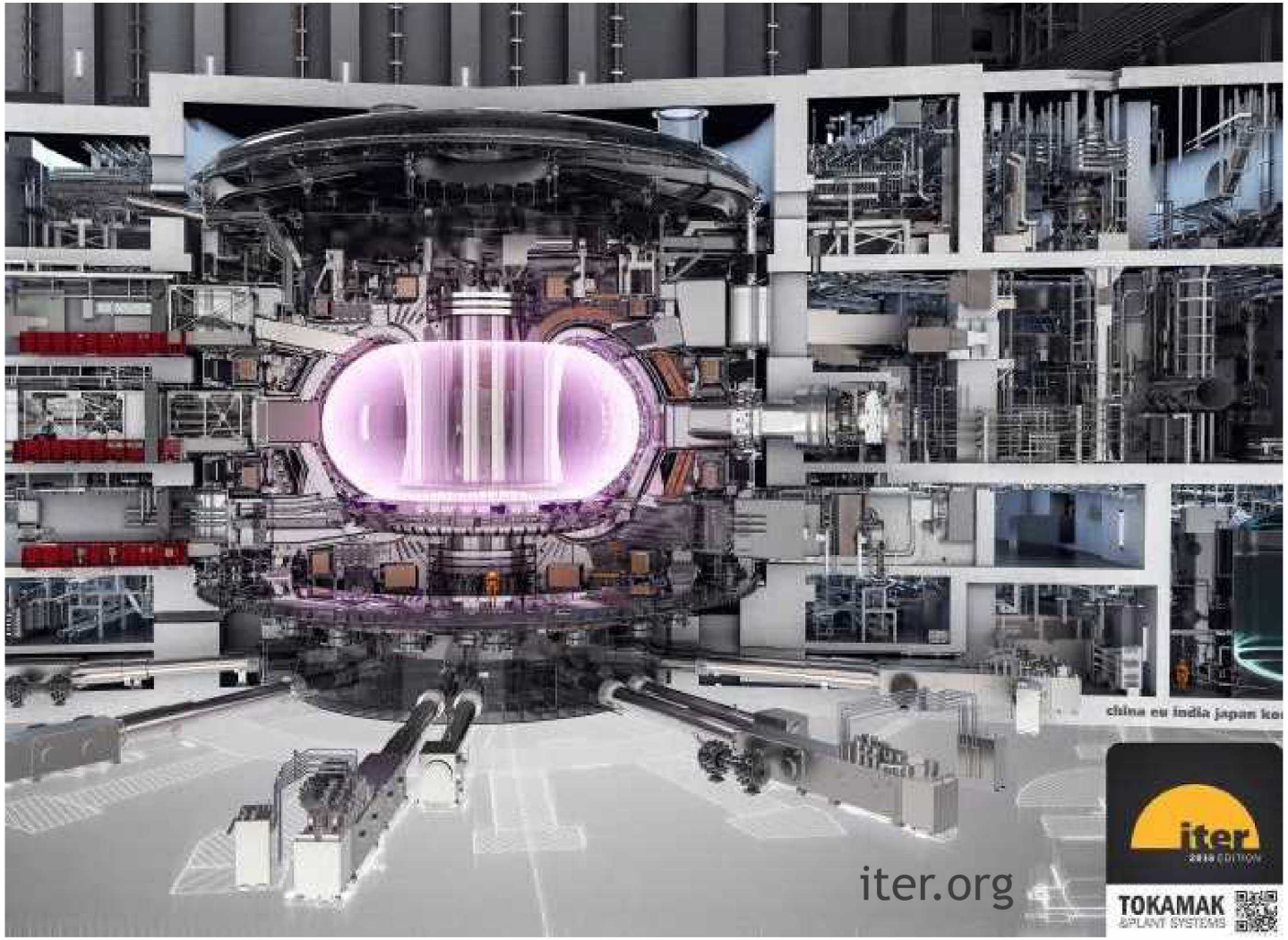




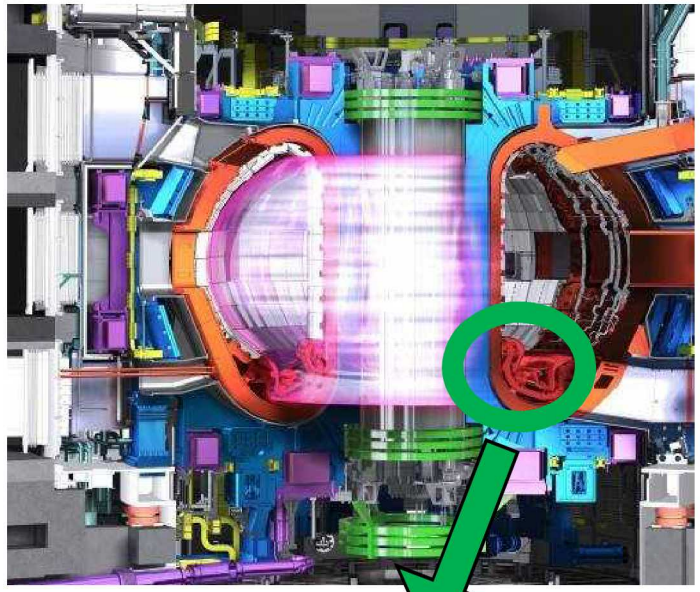
Fusion energy

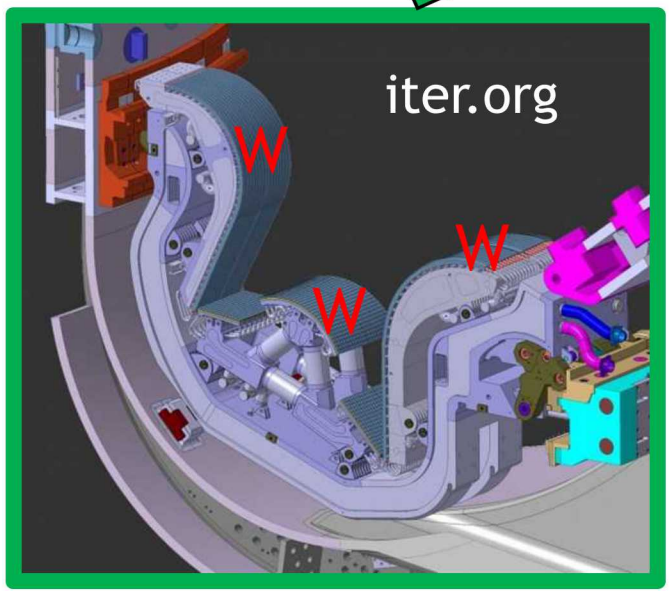
- relatively clean
- sustainable & abundant
- no risk of meltdown
- what materials can contain a hot fusion plasma?

ITER—final step before a DEMOnstration reactor



Hydrogen-Tungsten interactions in fusion reactors





Tungsten is a leading candidate material for fusion reactors

The divertor is a hydrogen (D and T) rich environment

Concerns arise from

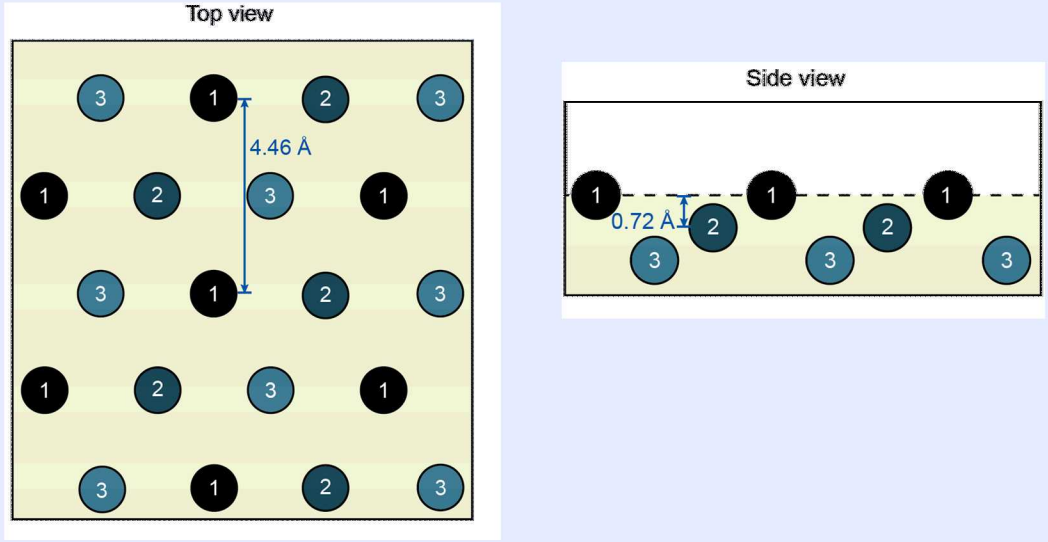
- hydrogen effects: embrittlement and blistering
- tritium retention and inventory

How does hydrogen adsorb on tungsten surfaces before diffusing into the bulk?

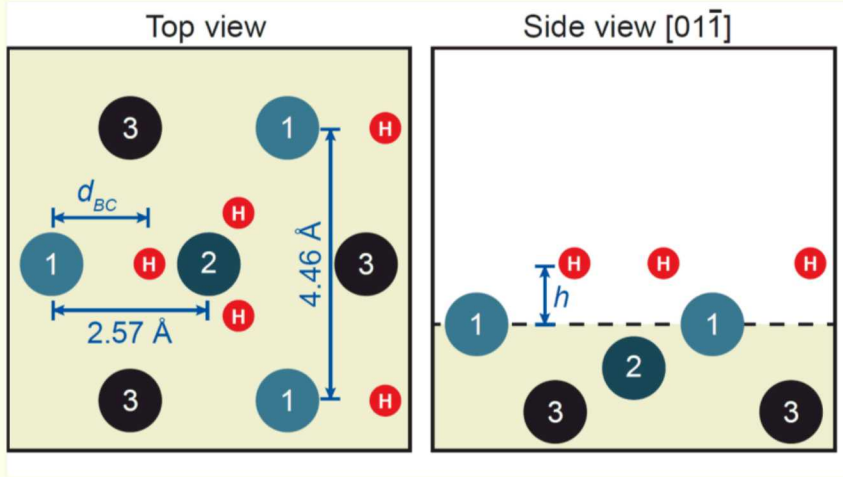
Hydrogen adsorption on tungsten surfaces

W(100) and W(110) have been studied, but W(111) is much more complex

W(111): open, corrugated surface structure



Complex H binding geometry predicted by DFT simulations [1]



1.5 Å ≤ d_{BC} ≤ 1.7 Å 0.95 Å ≤ h ≤ 1.10 Å

bond-centered (BC) site

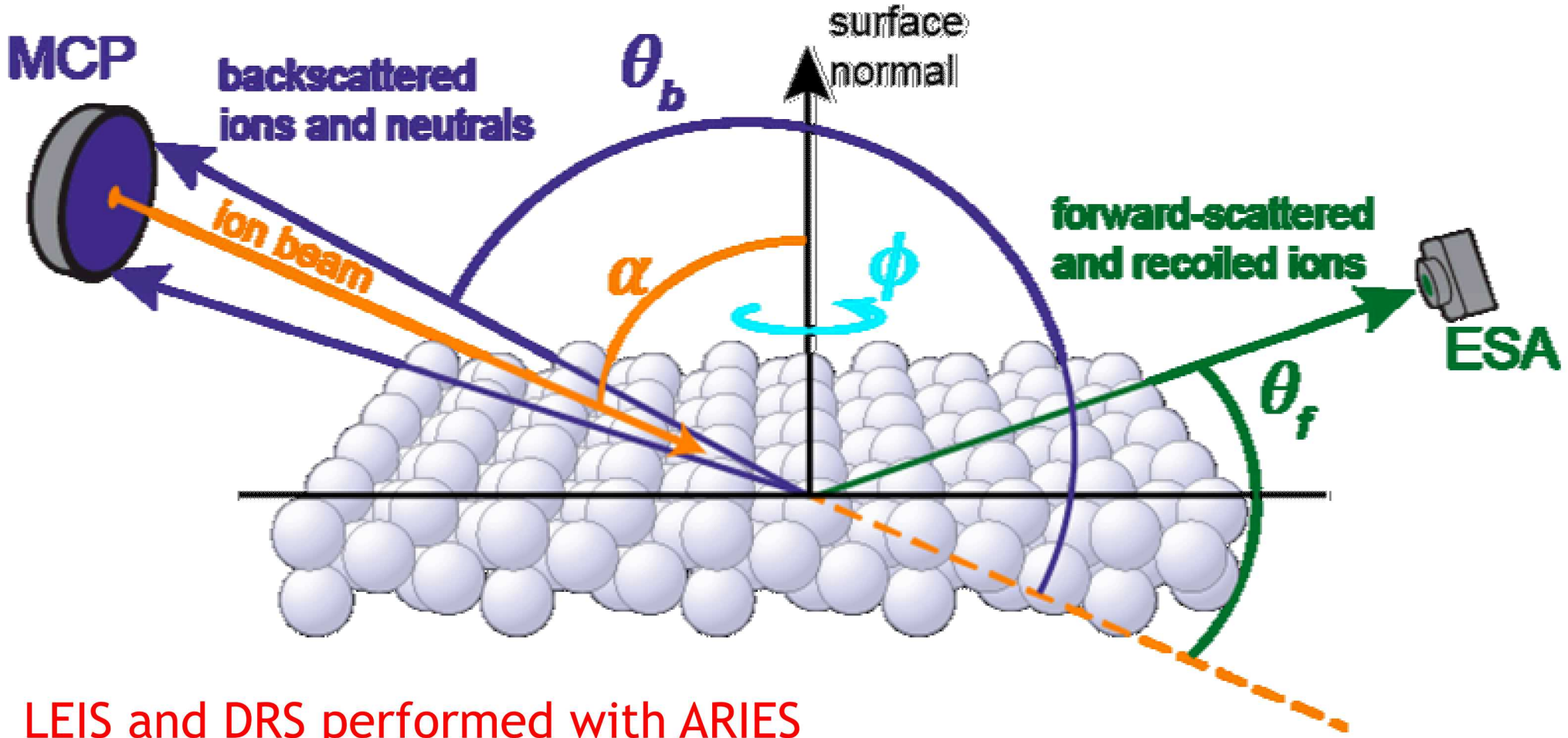
1. Characterize ion scattering off W(111)
2. Validate DFT prediction of BC site
3. Understand ion channeling on W(111)

[1] Z. Bergstrom et al., J. Phys.: Condens. Matter, (2019).

Characterizing W(111)+H(ads) system

LEIS, DRS, and ICISS

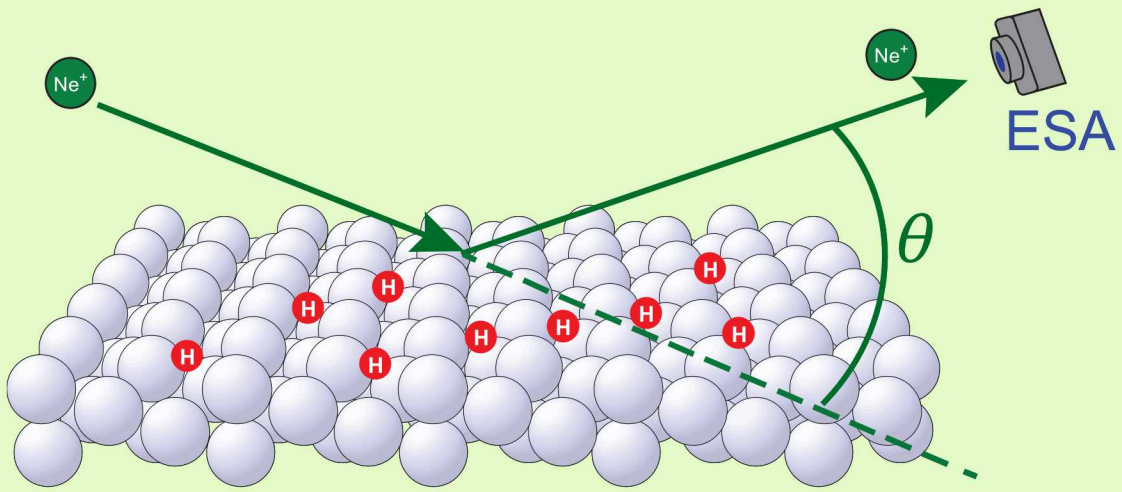
ARIES: Angle-Resolved Ion Energy Spectrometer



- LEIS and DRS performed with ARIES
- can also be configured for backscattering measurements

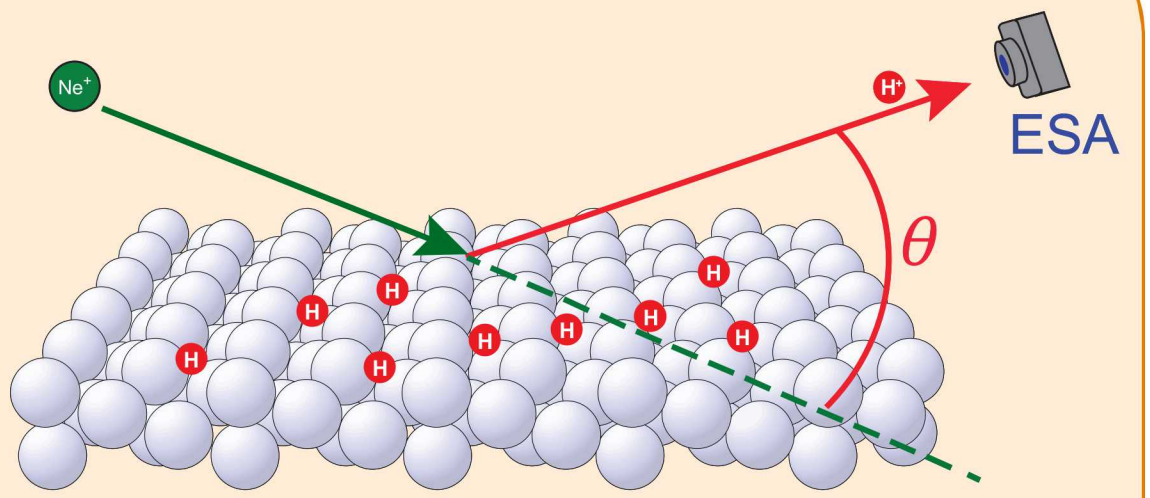
LEIS and DRS

Low energy ion scattering (LEIS)



$$\frac{E}{E_0} = \left(\frac{\cos\theta \pm \sqrt{\mu^2 - \sin^2\theta}}{1+\mu} \right)^2$$

Direct recoil spectroscopy (DRS)



$$\frac{E}{E_0} = \frac{4\mu}{(1+\mu)^2}\cos^2\theta$$

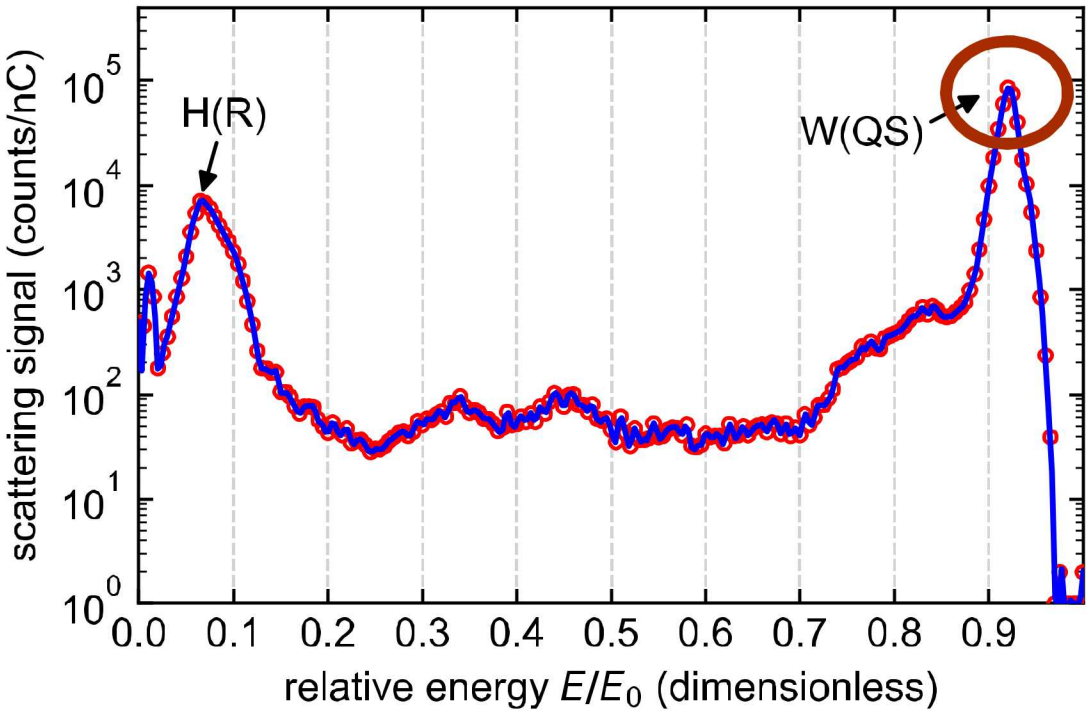
- both techniques can be performed simultaneously
- energy of detected ion depends only on μ and θ

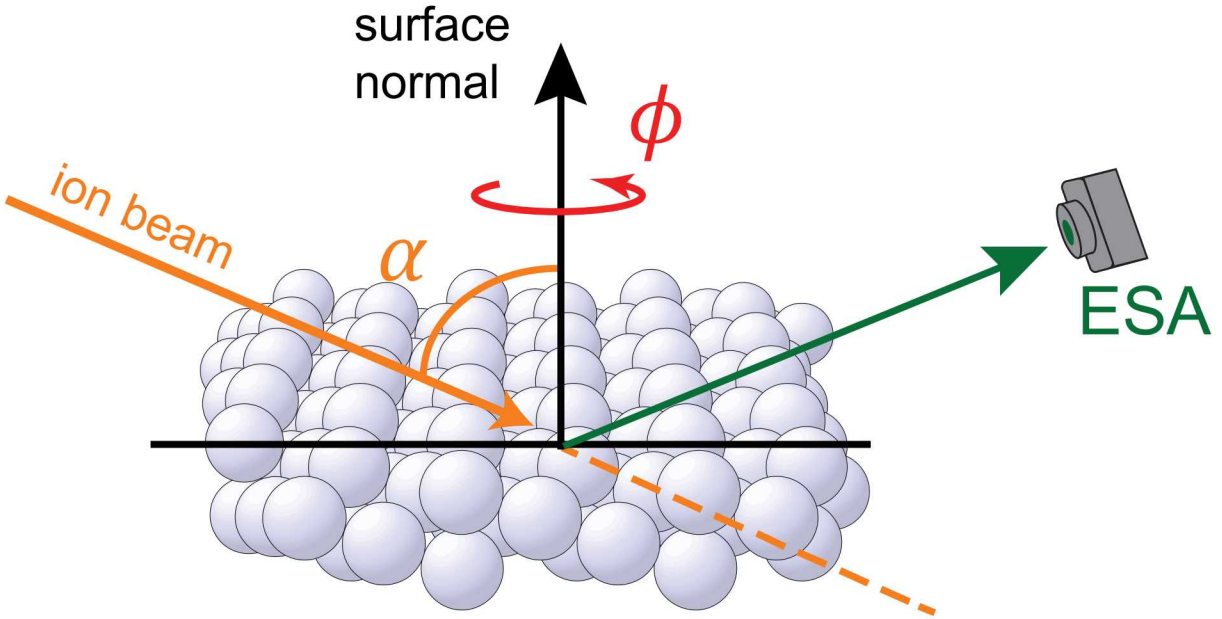
$$\mu = \frac{m_T}{m_P}$$

Multi-layer scattering from W(111) substrate

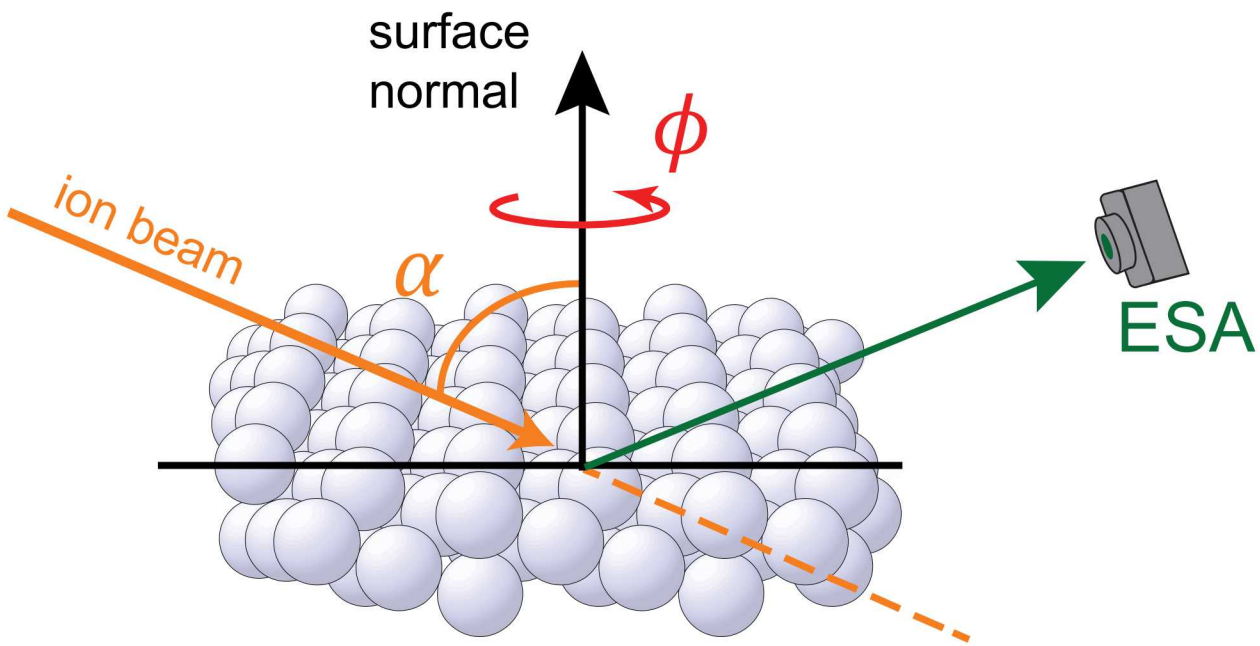
Constructing multi-angle scattering maps with LEIS

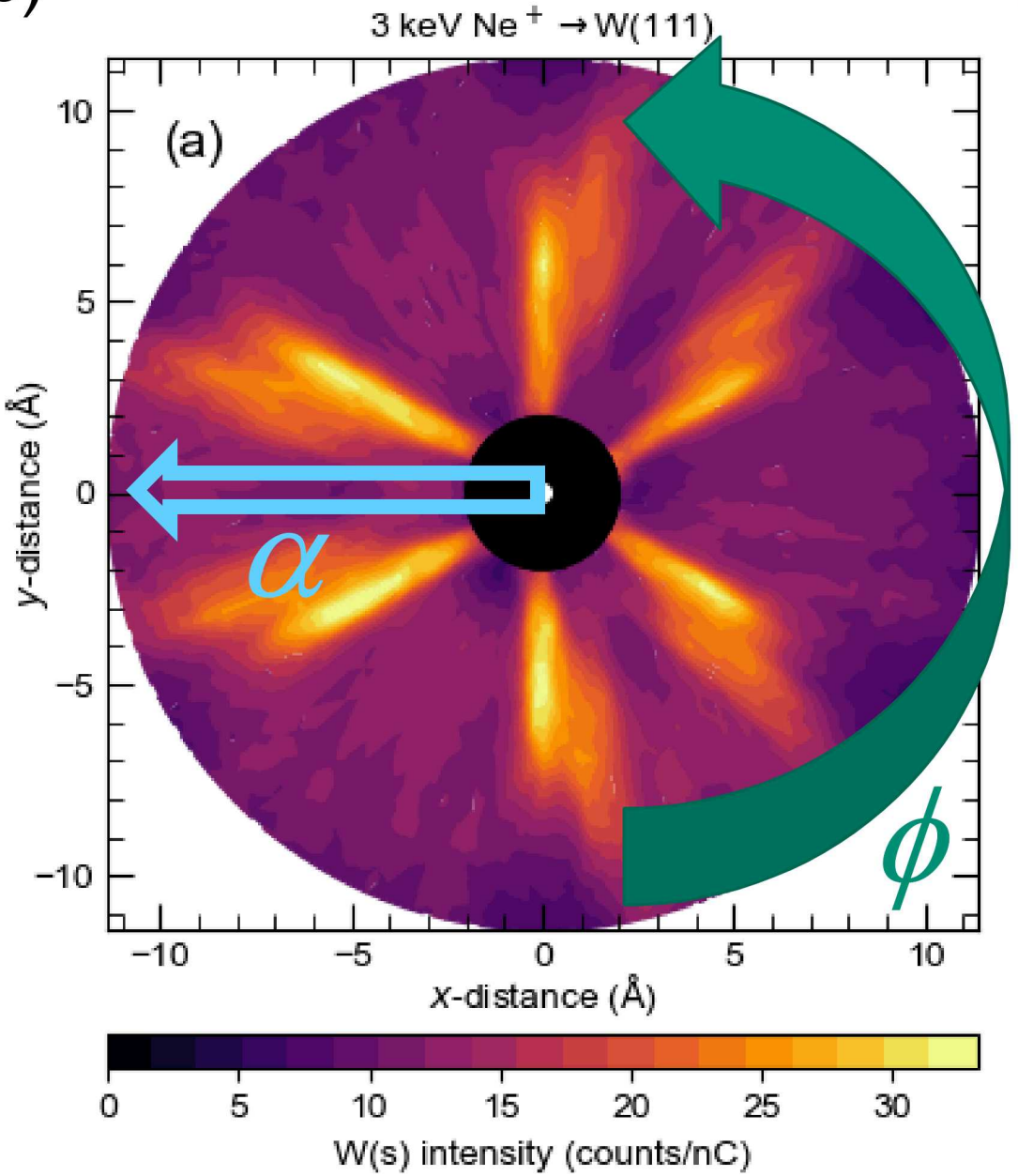
track counts of scattered Ne^+ while varying angles α and ϕ



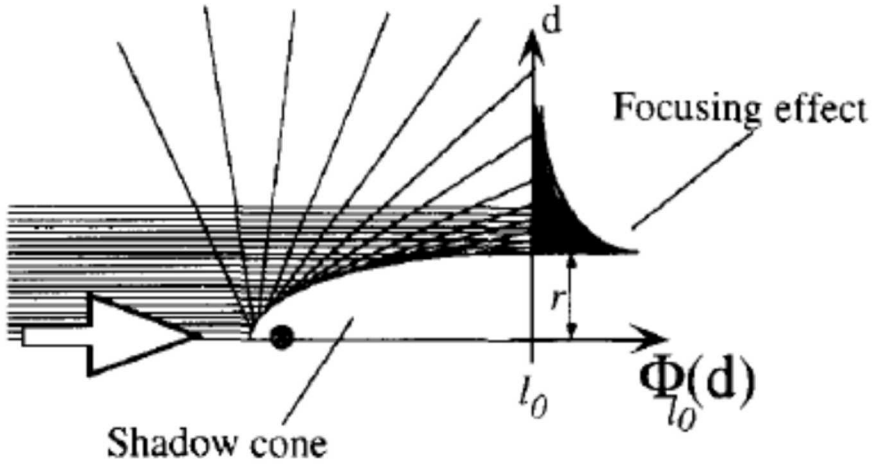


Multi-angle scattering maps for W(QS)

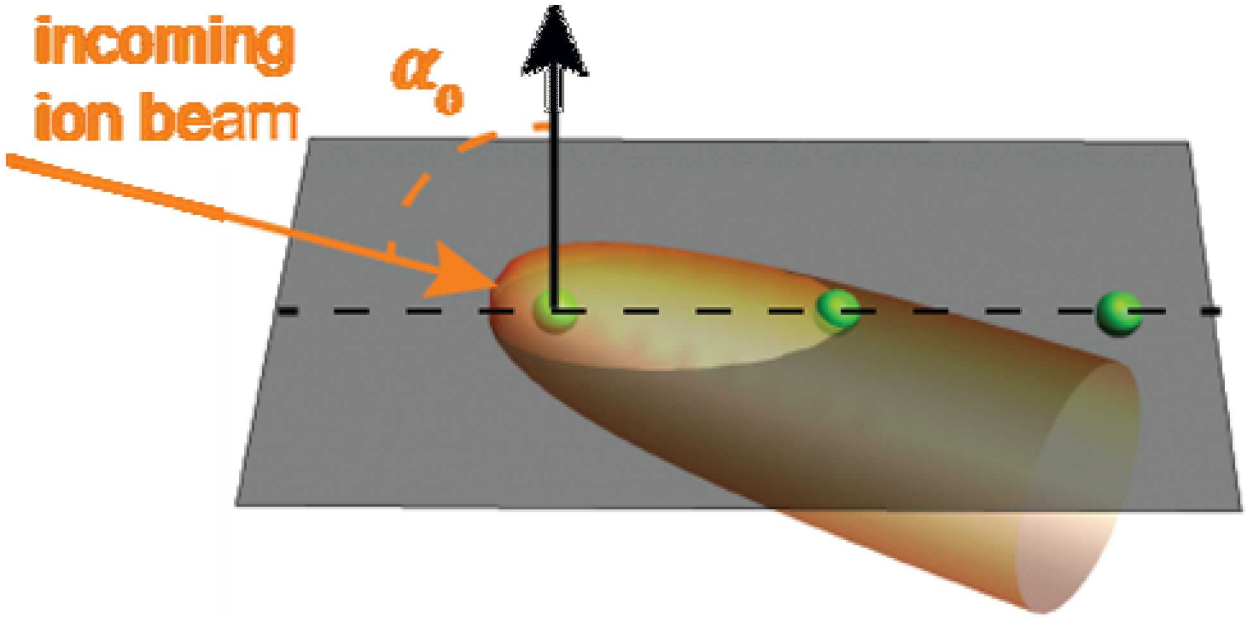




Shadow cones

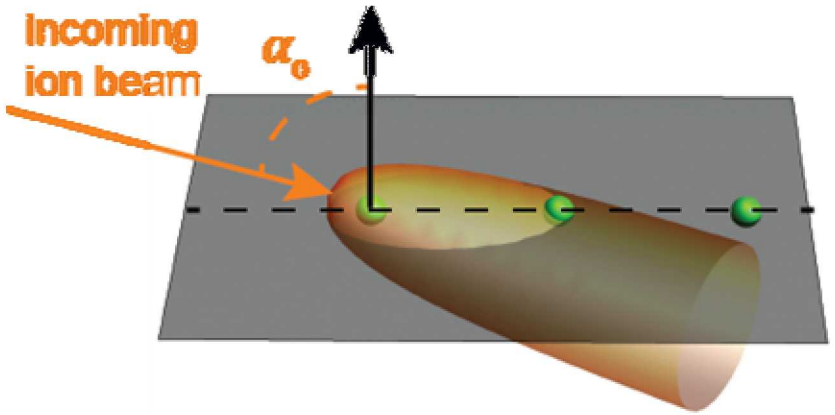


Agostino et al., Surf. Sci. **384,** (1997).

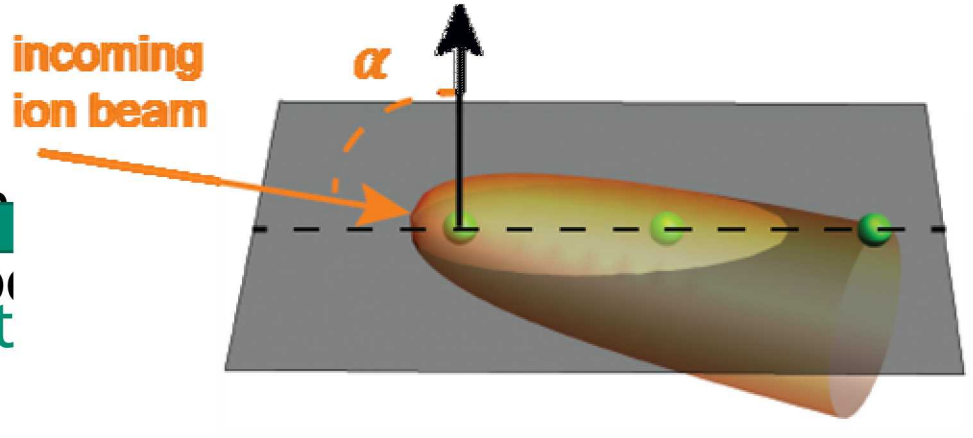


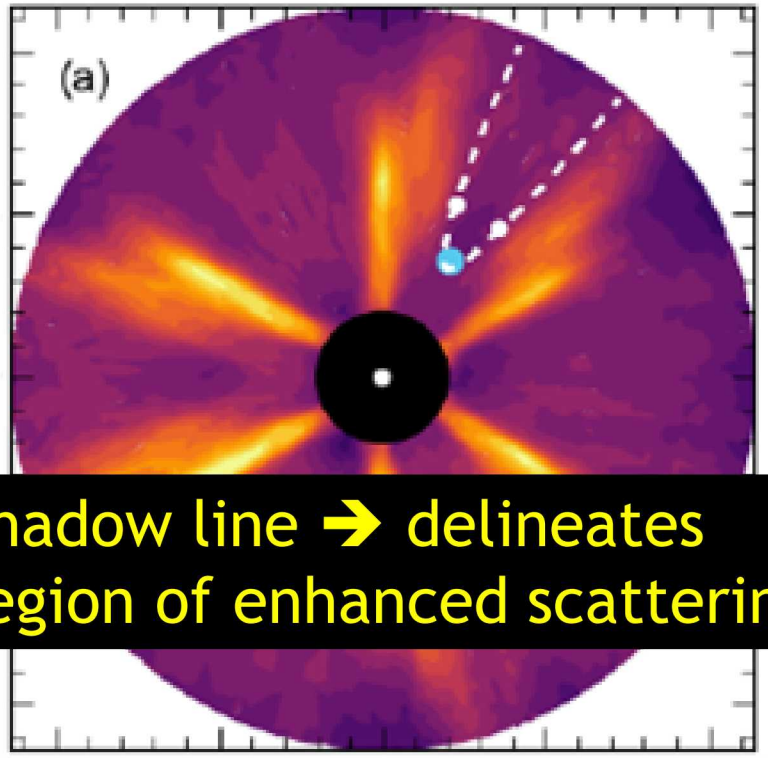
- Shadow cone arises from ion focusing
- Enhanced scattering or recoil signal when cone coincides with neighboring atom

Shadow line analysis



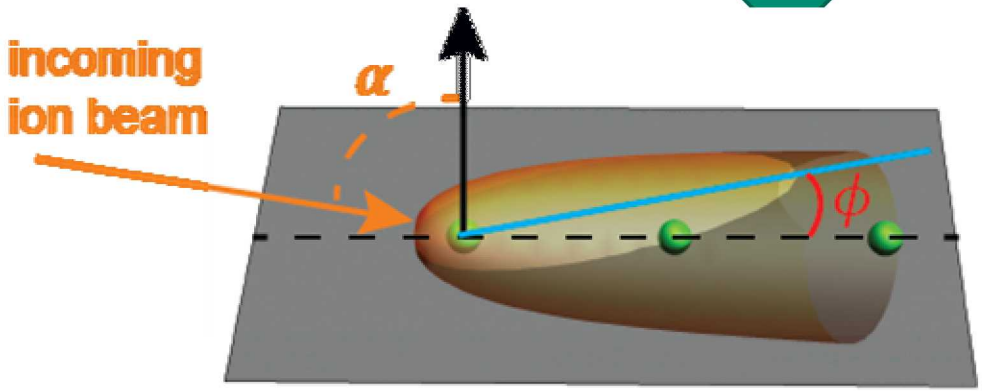
L[redacted]
coincides with neighb
shadow cone overshoot
neighbor for larger α





Shadow line ➔ delineates region of enhanced scattering

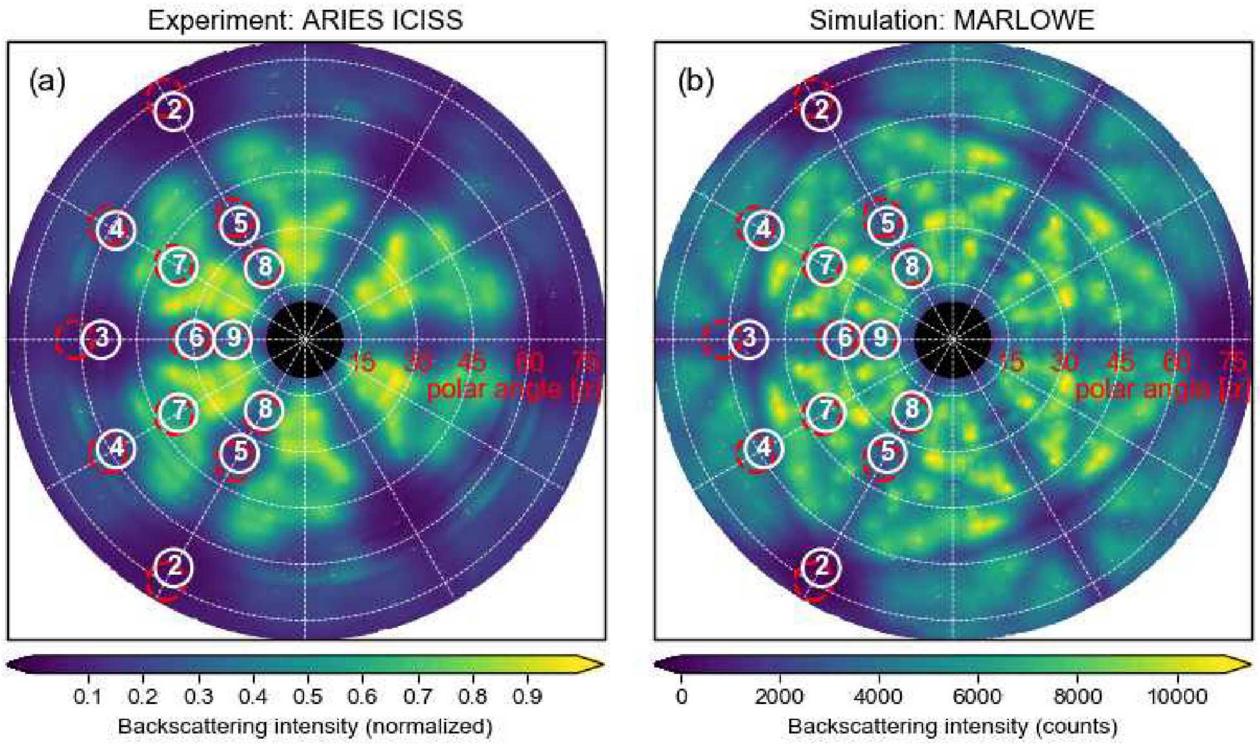
edge of cone realigned by ϕ rotation

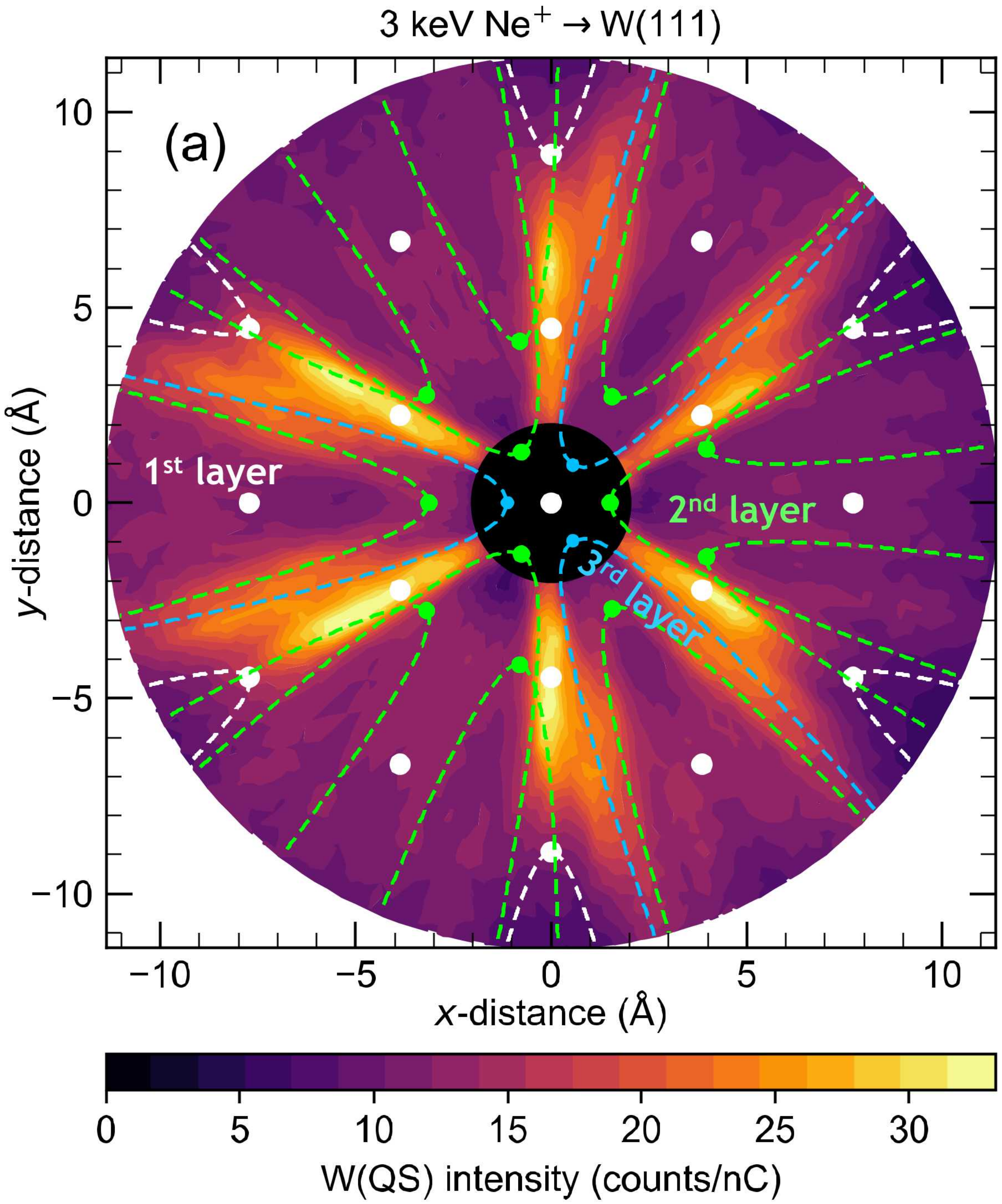


Agostino et al., Surf. Sci. **384,** (1997).

Shadow lines for three W layers

- Getting closer... can the scattering signal near the center be explained?
- Crystalline orientation confirmed with ICISS backscattering maps

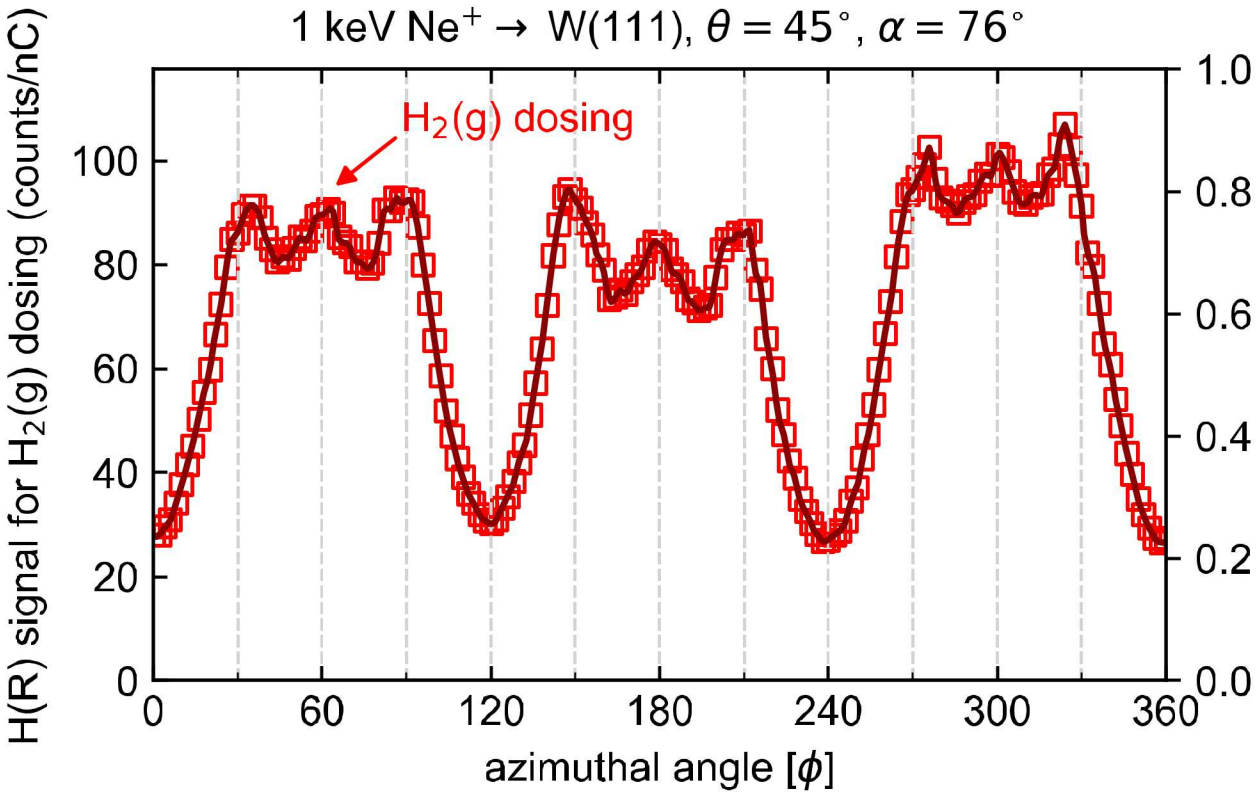


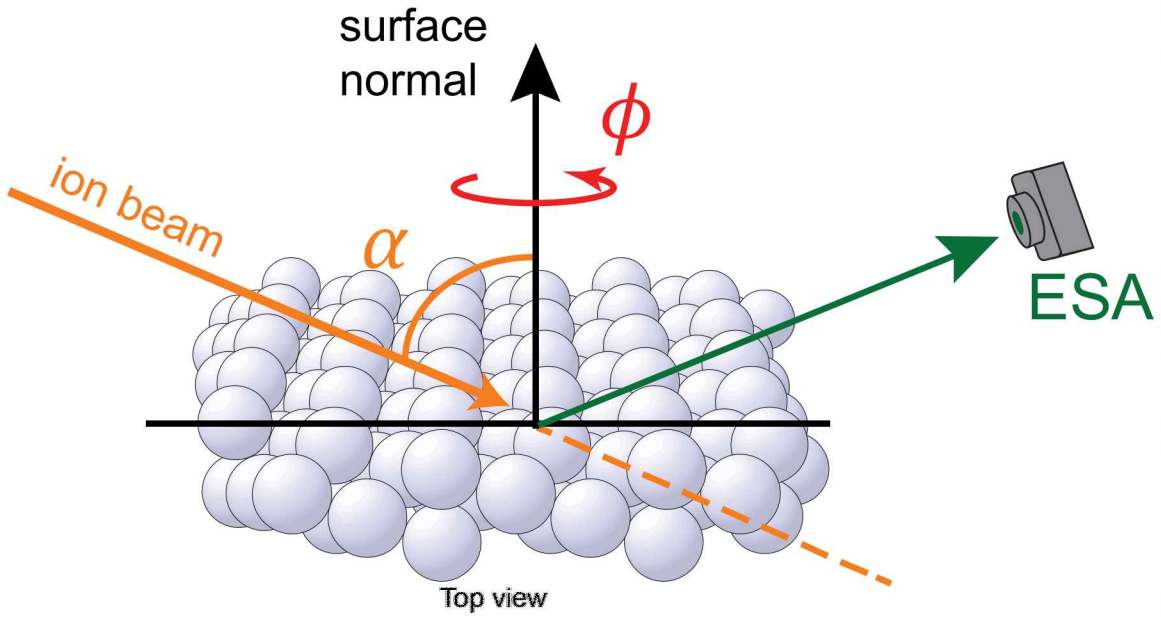


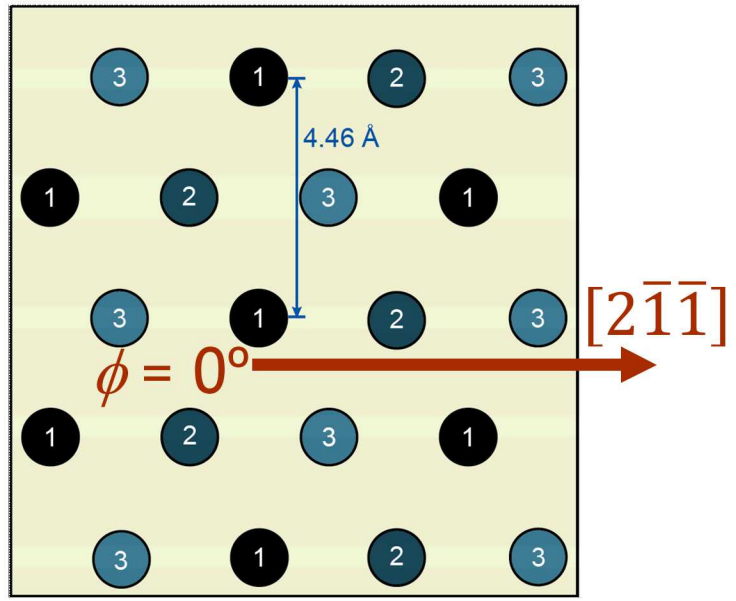
Determination of H adsorption sites on W(111):

modeling DRS measurements with MD simulations

DRS measurement of H at a single α

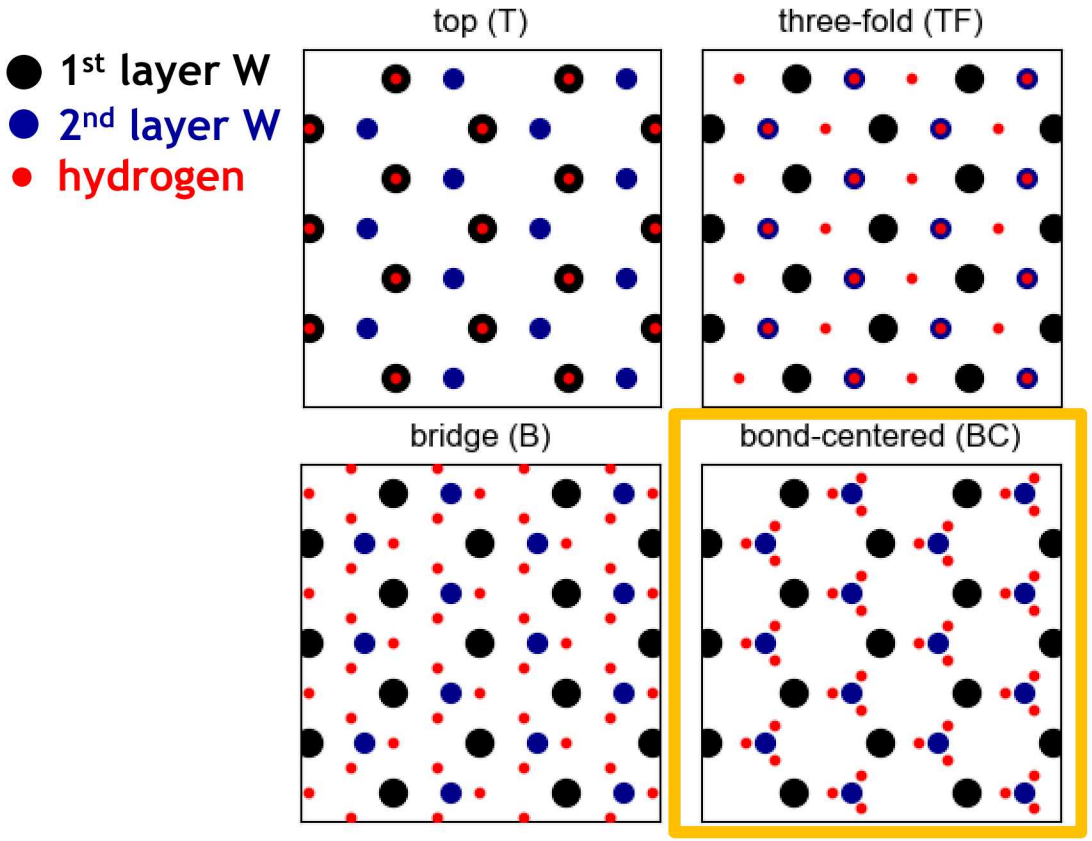




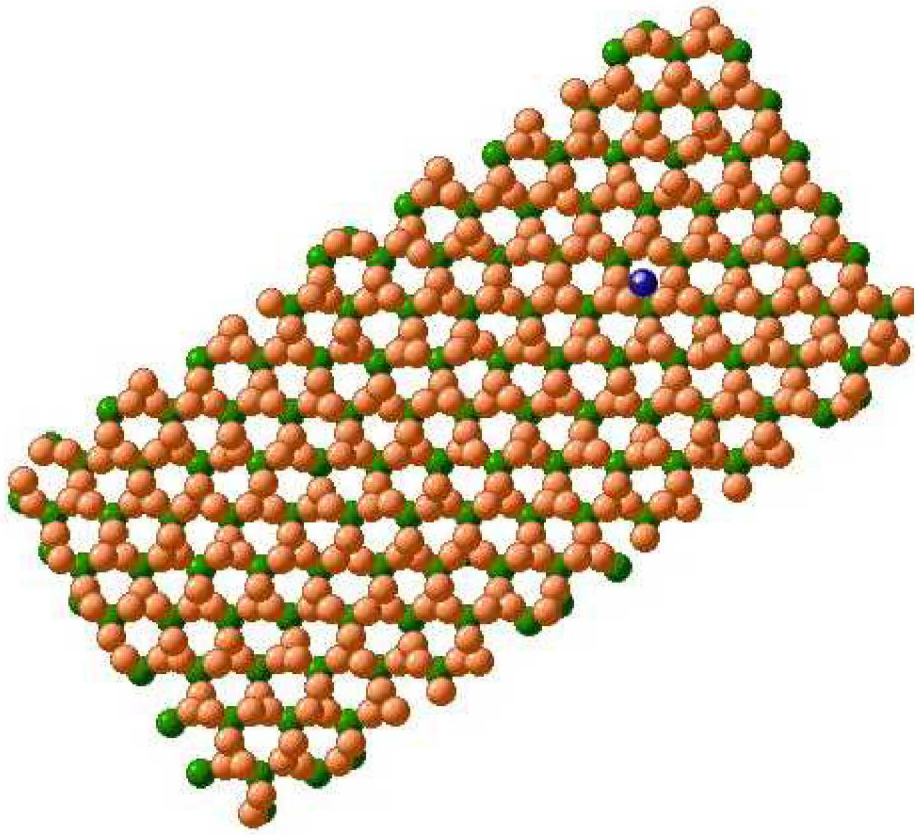


Molecular dynamics (MD) simulations with Kalypso [2]

Simulations performed for the DFT predicted BC site as well as 3 other high symmetry sites for comparison

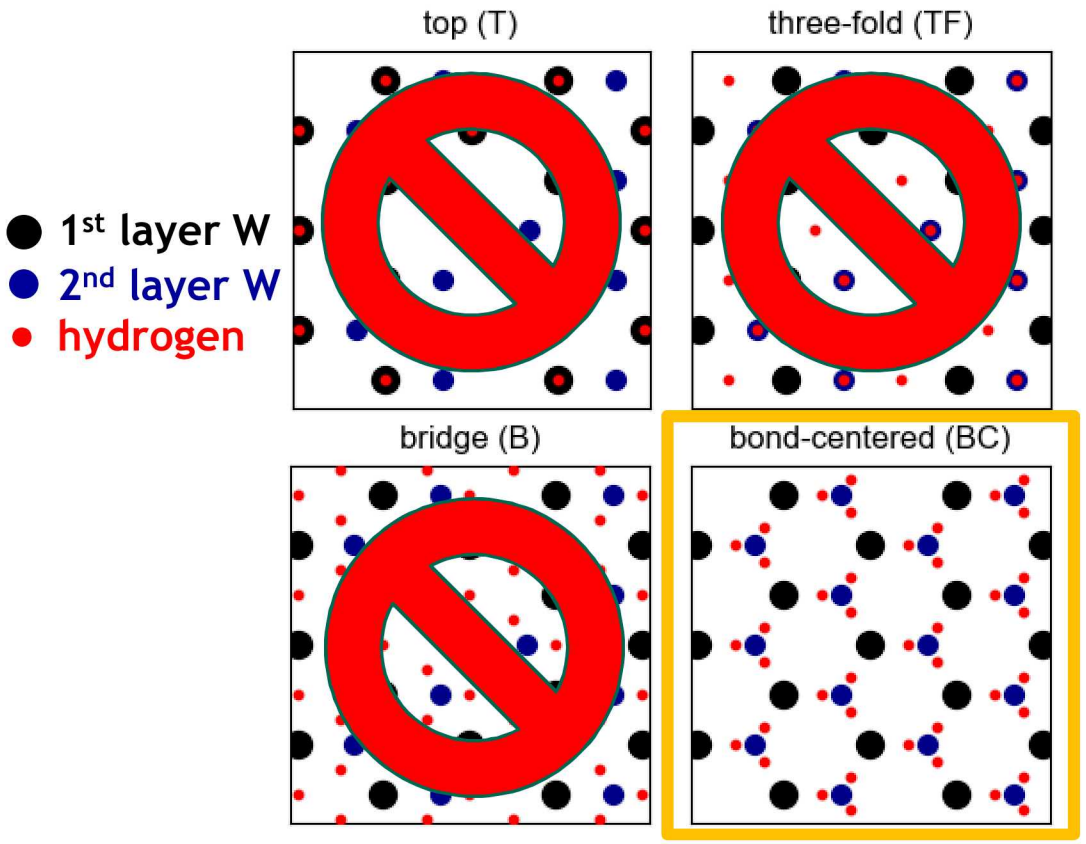


DFT prediction

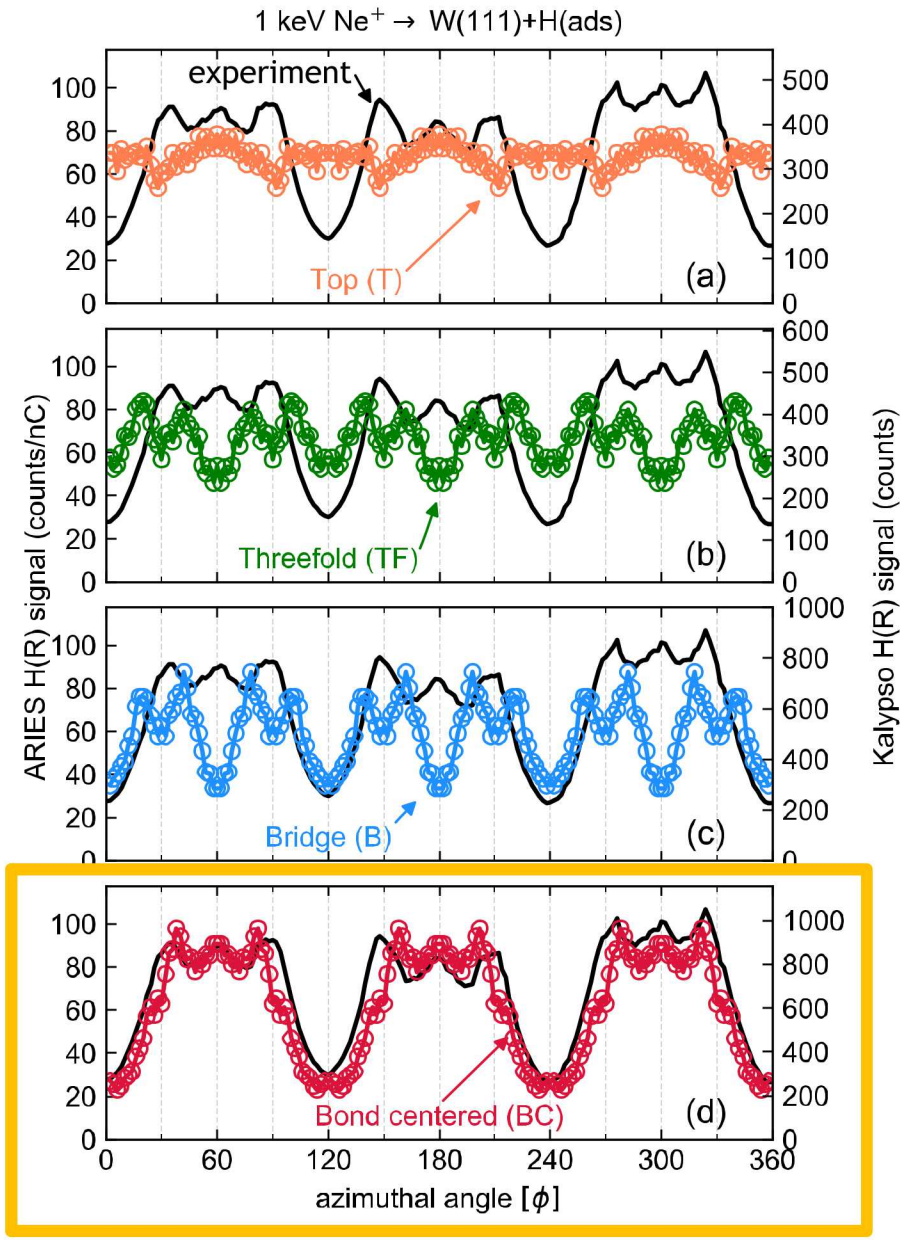


[2] Karolewski, Nucl. Instrum. Methods Phys. Res. B **230,** (2005).

MD simulation results compared to experimental H(R)



DFT prediction



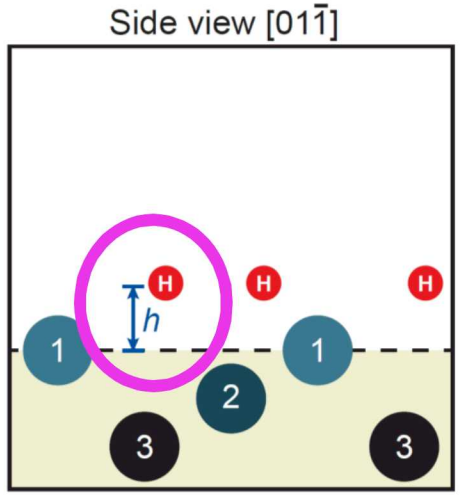
Constraining adsorbate height and position

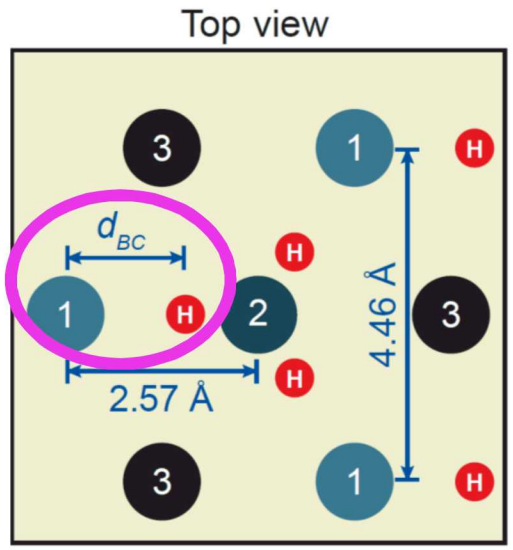
h = 1.0 ± 0.1 Å

DFT prediction:
0.95 Å ≤ h ≤ 1.10 Å

d_{BC} = 1.6 ± 0.1 Å

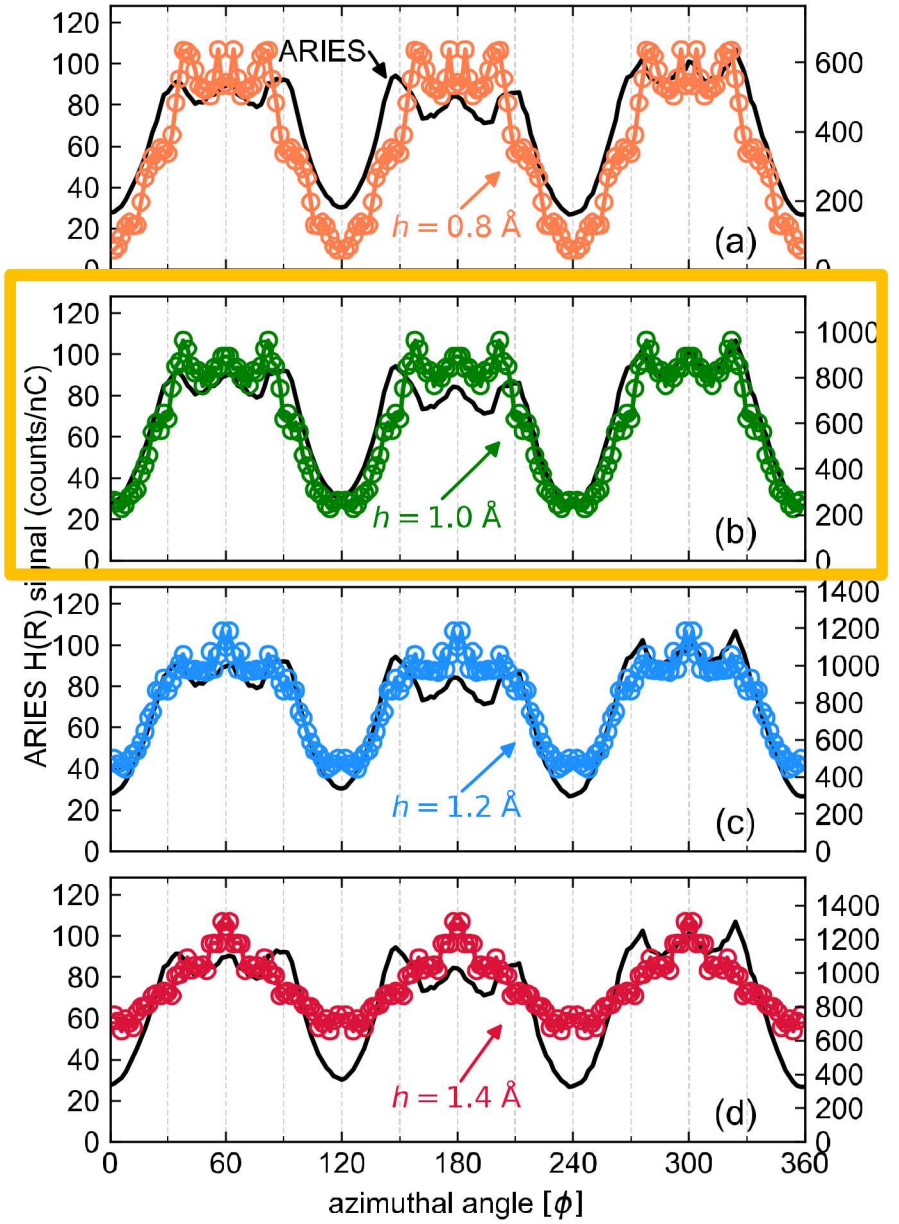
DFT prediction:
1.5 Å ≤ d_{BC} ≤ 1.7 Å





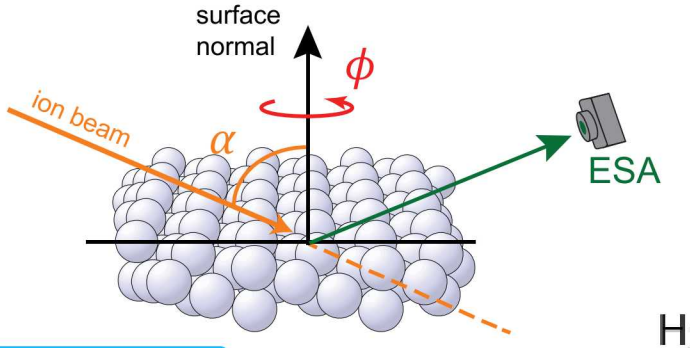
DFT prediction

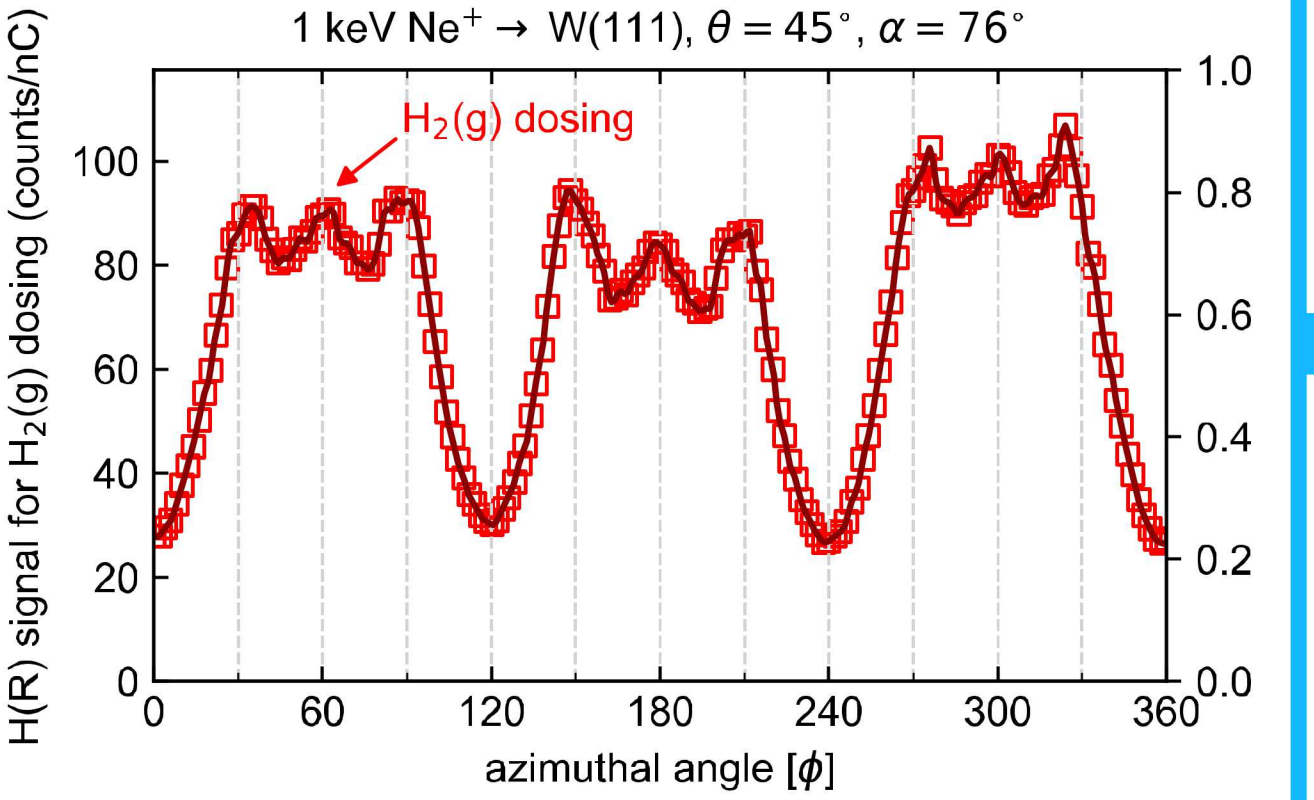
varying h

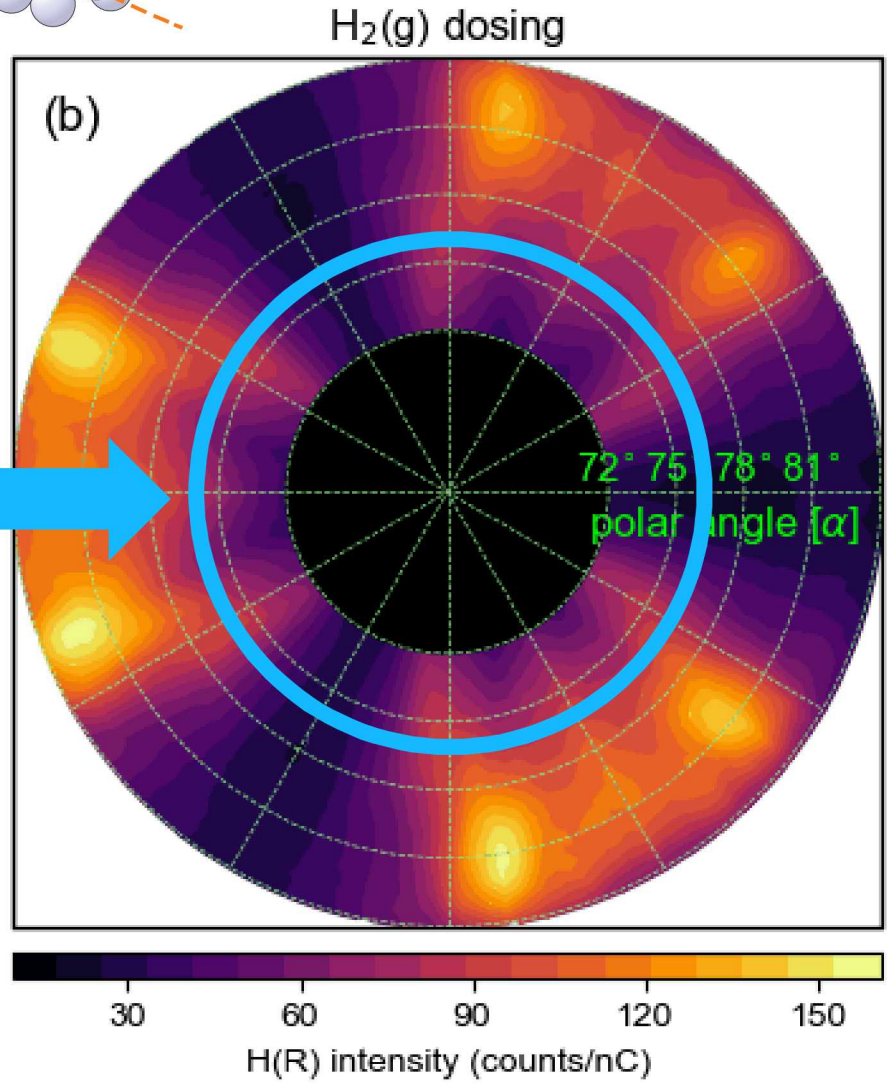


Ion channeling for the W(111)+H(ads) system

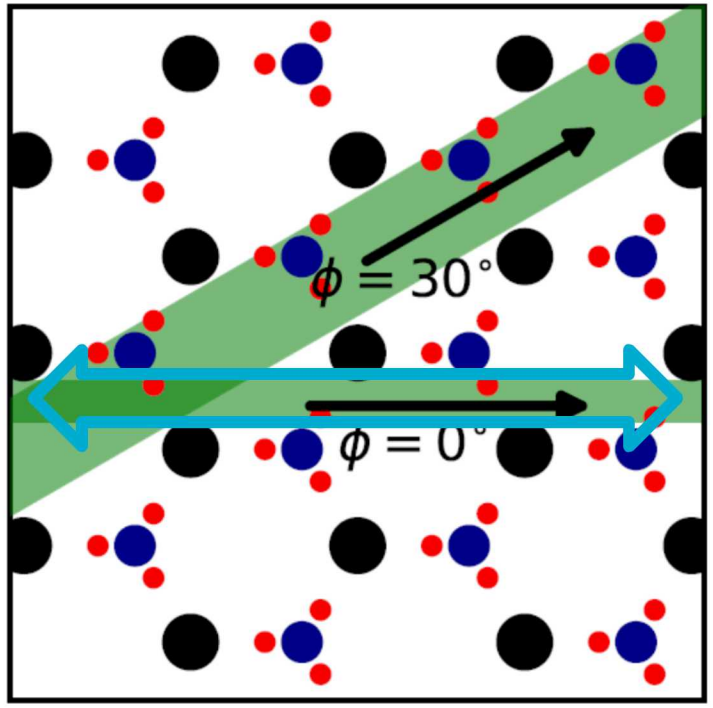
Constructing H(R) maps

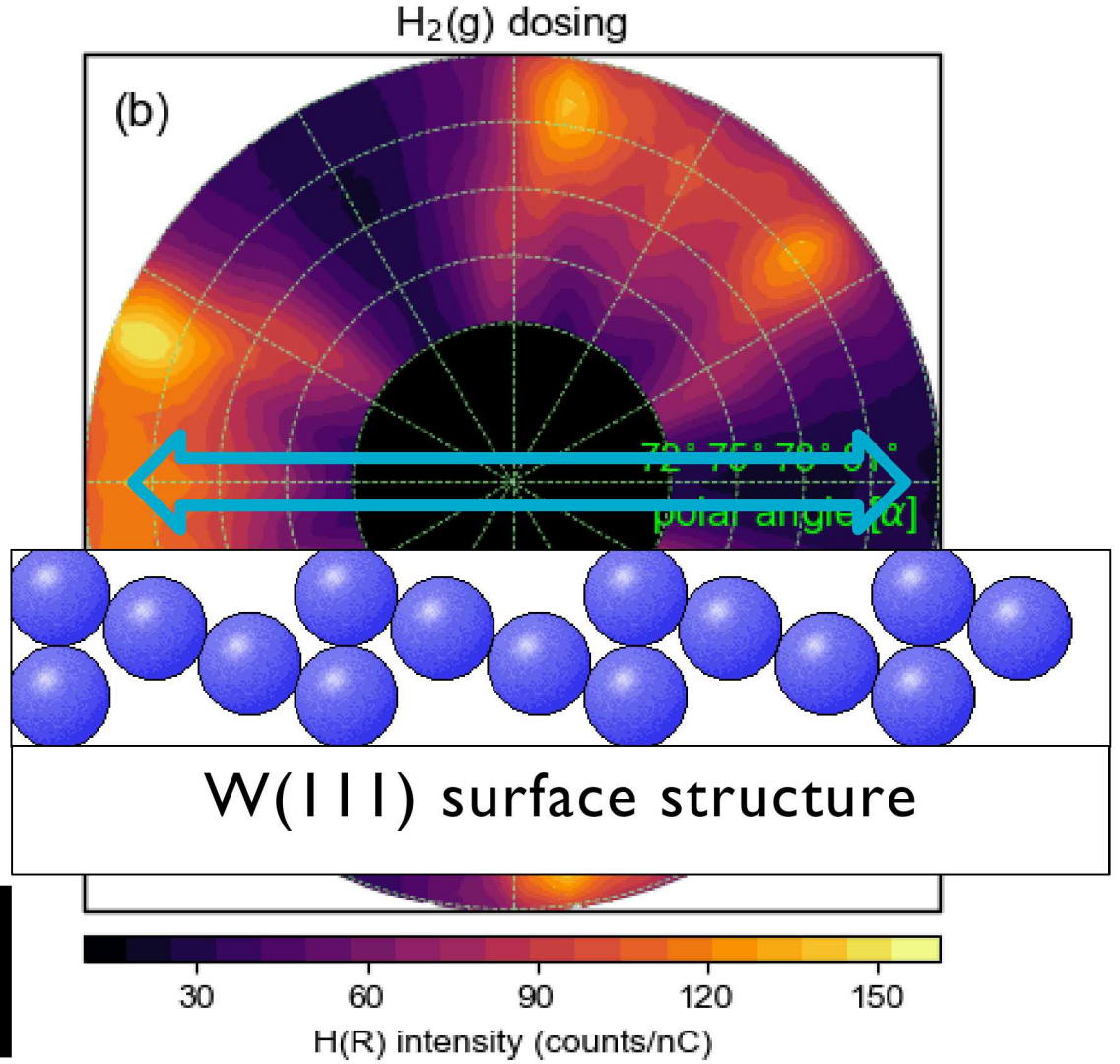






Ion channeling along and into W(111) surface

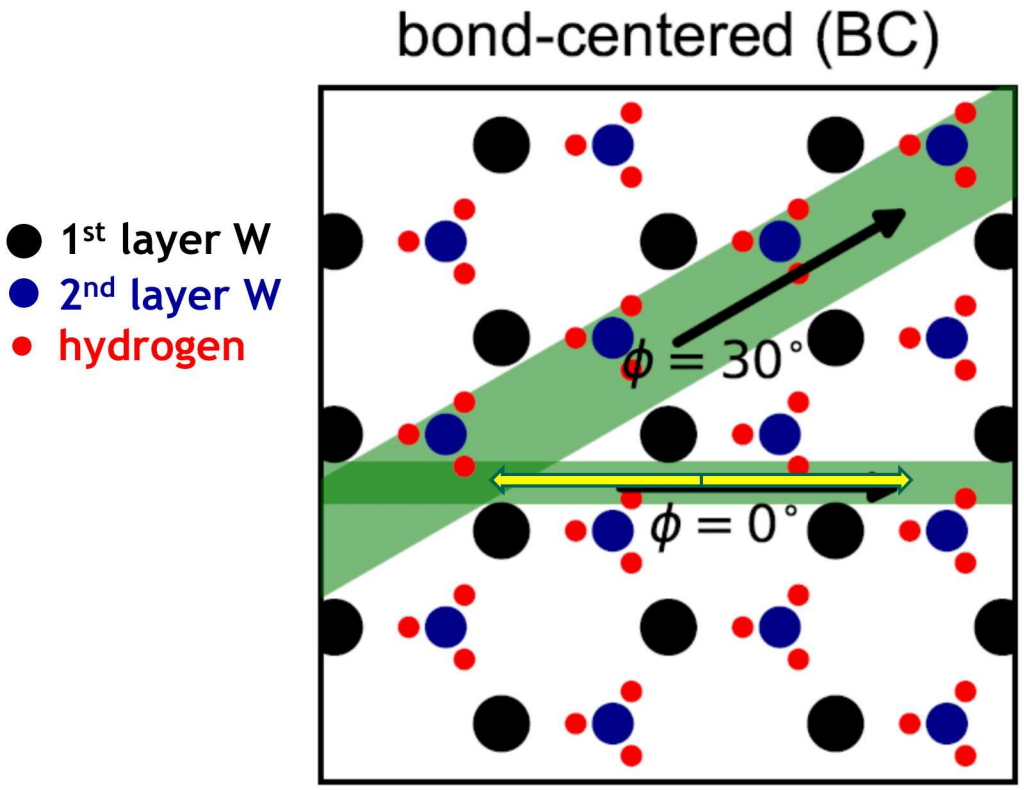


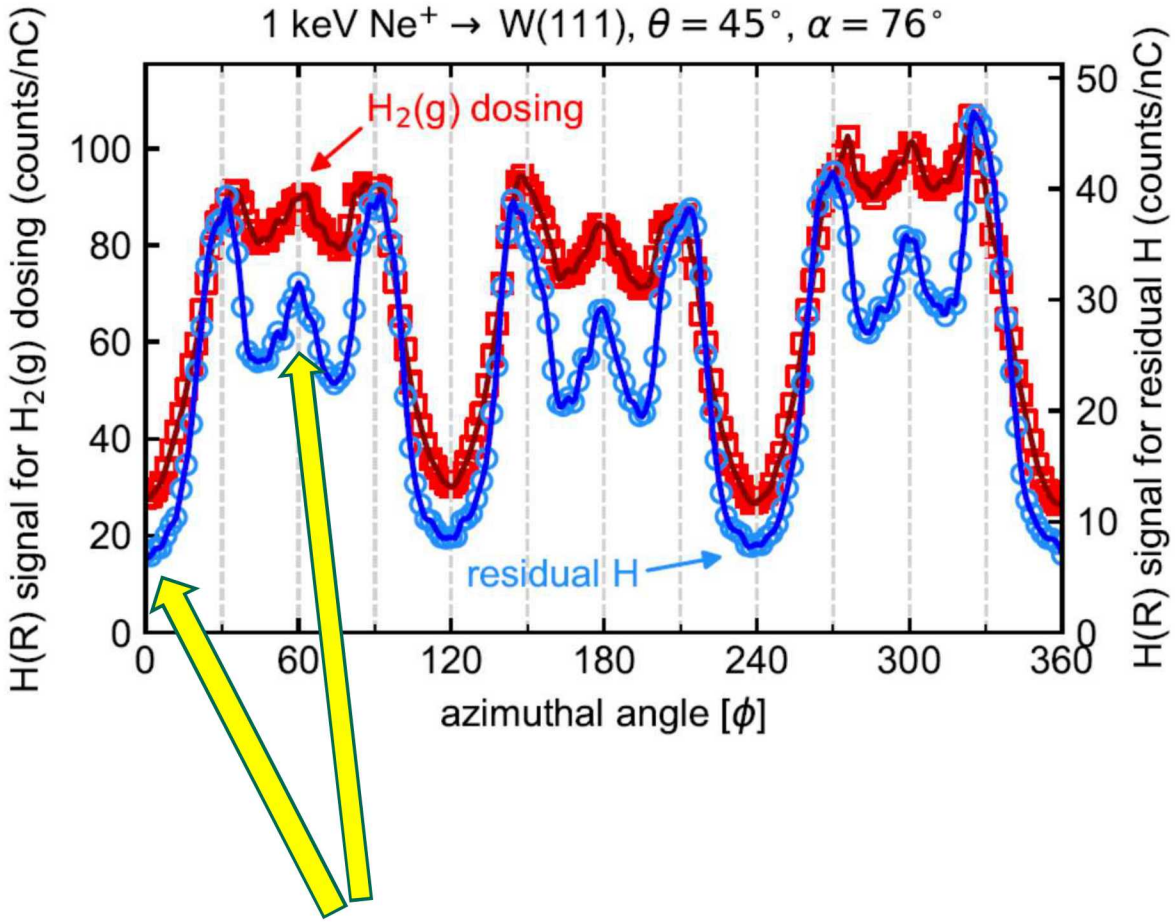


Previous studies [3]:
H within channel ➔ peak in H(R) signal

[3] Kolasinski et al., PRB, (2012).

Enhanced ion channeling due to adsorbed H





Increased signal with H dosing due to enhanced ion channeling

Summary of W(111)+H(ads) study

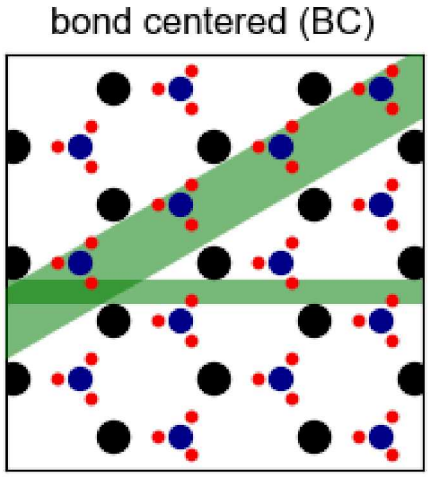
1. Advanced existing analysis and modeling techniques for surface hydrogen detection:

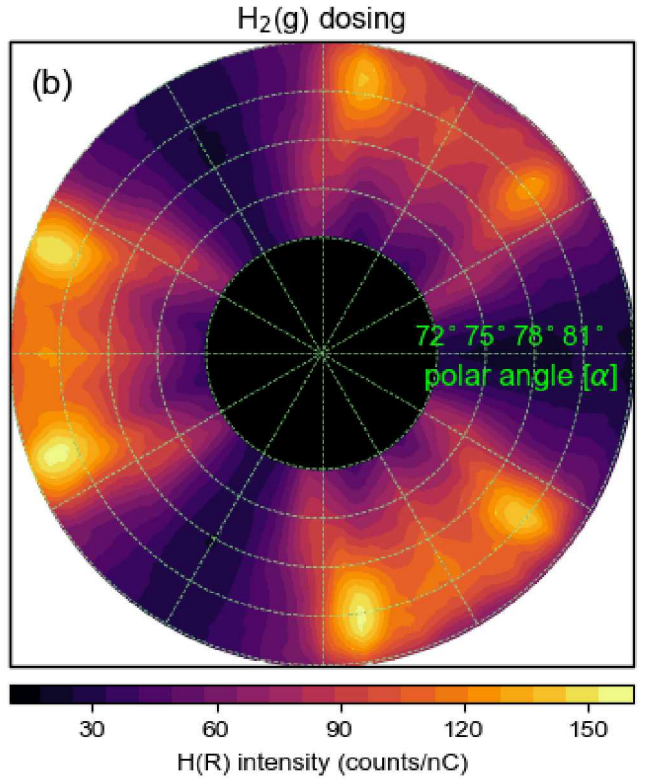
   complex binding geometry and corrugated surface

2. Validated DFT predictions:

   DFT provides inputs for larger scale models, e.g.

   - interatomic potentials for MD
   - hydrogen dissociation energies on surfaces





Extra slides

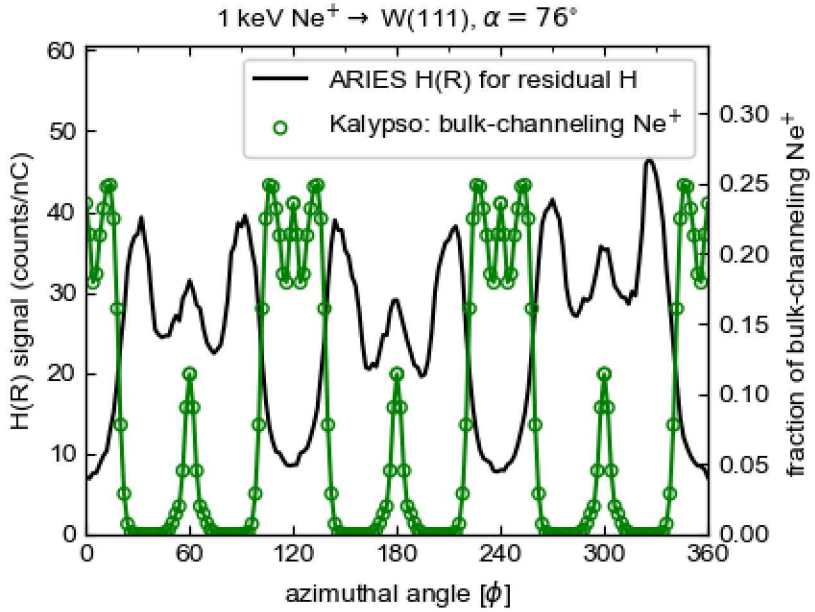
Modeling H(R) with molecular dynamics (MD) simulations

physics included	assumptions made
saturated H coverage on W substrate	elastic collisions—universal ZBL potential
surface relaxation of W substrate*	only include projectile—target interactions
vibrational displacements of W & H*	stationary target atoms
only count recoiled H with final trajectory and energy that corresponds to detector	damage to target was not tracked

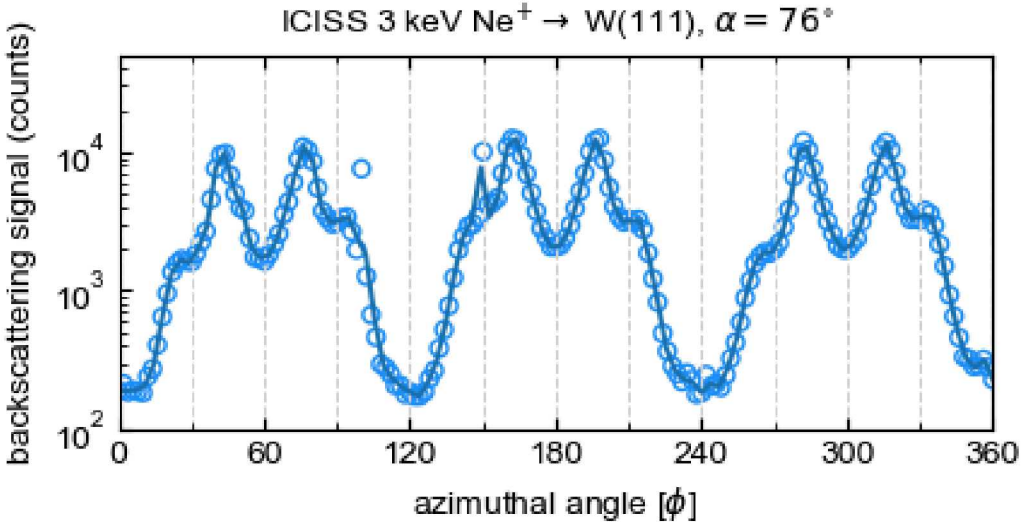
*DFT calculations performed by collaborators at U. Tenn

Channeling into the surface breaks symmetry

MD simulation data



Experimental data



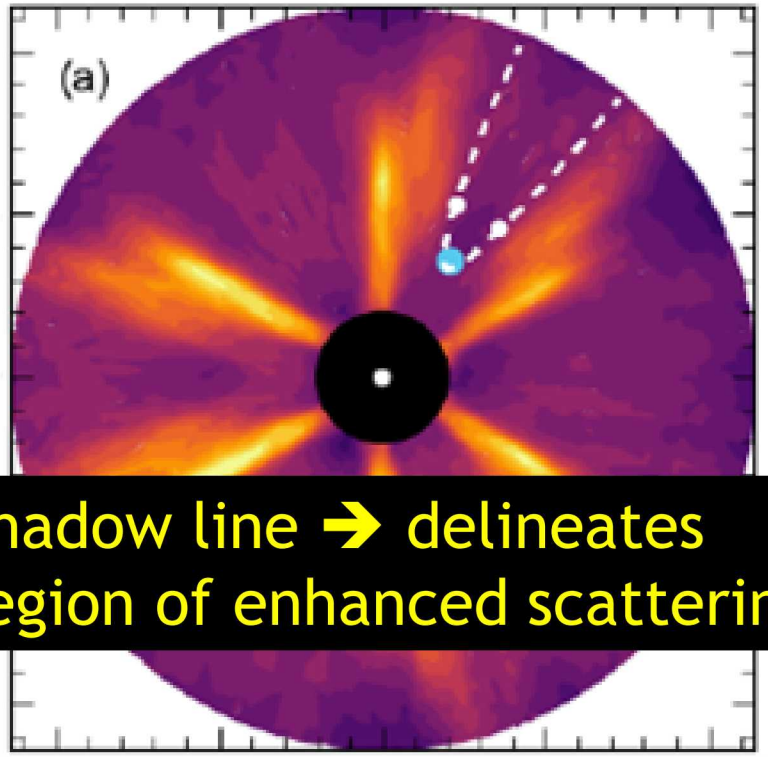
Channeling into surface correlate to H(R) minima

ICISS minima = maximum channeling into surface

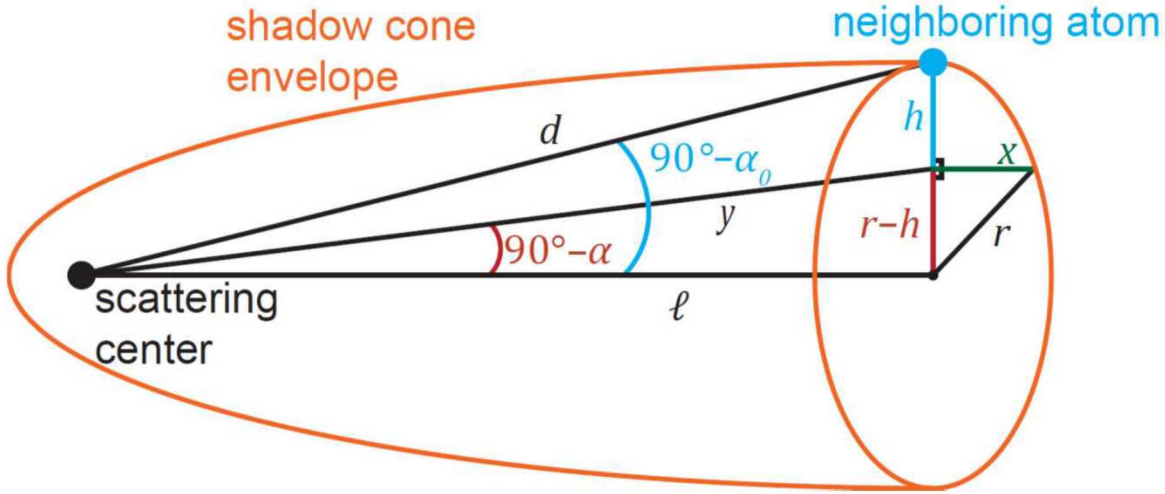
Shadow lines—analytic description

- In the literature, shadow lines were calculated numerically
- I showed that shadow lines can be determined analytically, based on geometrical arguments:

$$\phi_{rot} = \arctan\left[\cot(\alpha_0)\sqrt{1-\frac{\cos^2(\alpha)}{\cos^2(\alpha_0)}}\right]$$



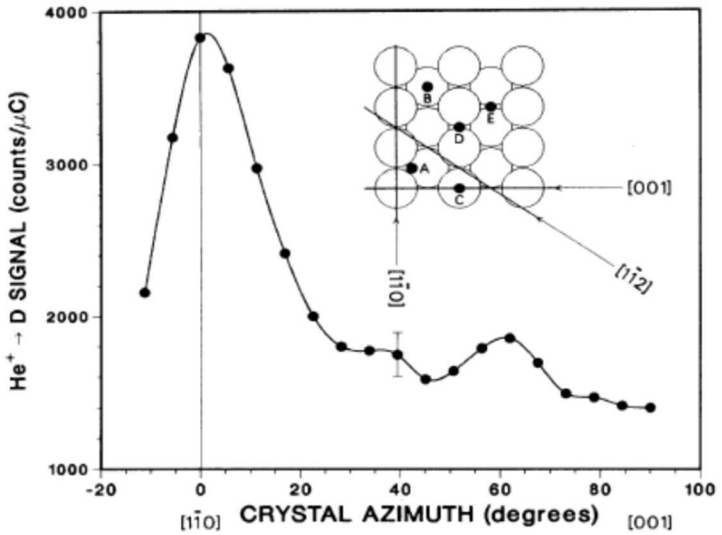
Shadow line ➔ delineates region of enhanced scattering



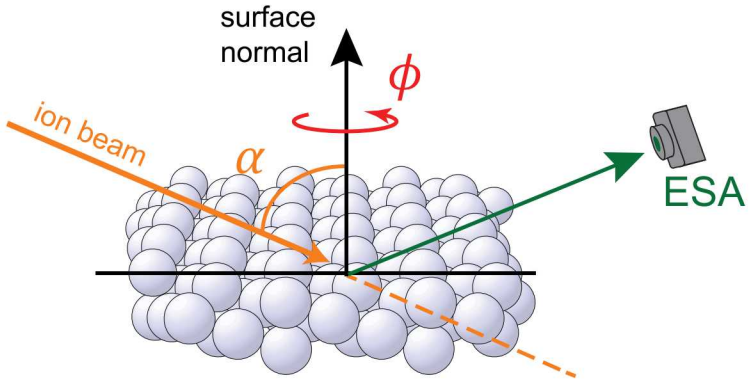
Early study to find H on surfaces—shadow cone analysis

LEIS to detect D on Pd surface

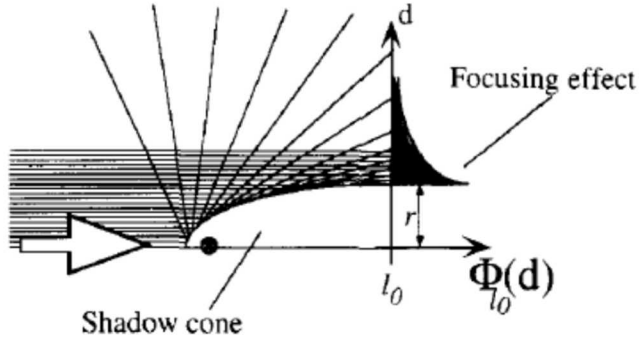
Bastasz et al., Phys. Rev. Lett. **63**, (1989).



D scattering signal, varying only ϕ

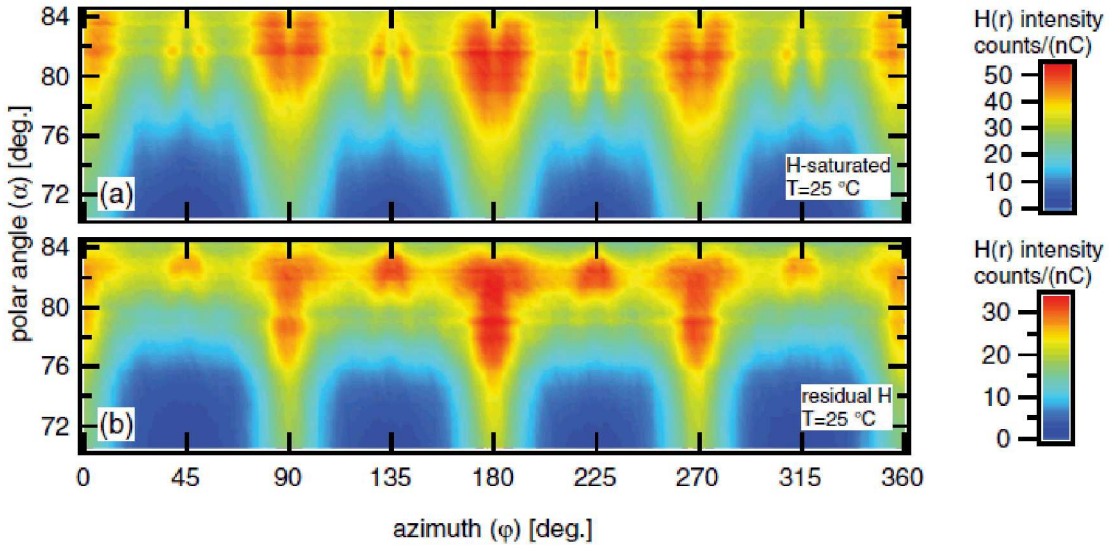


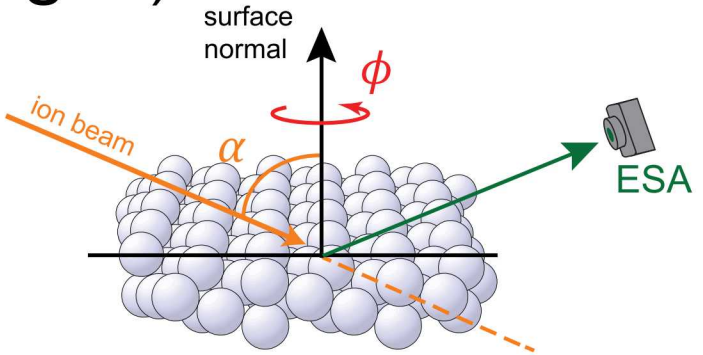
- based on D being hidden by Pd-atom shadow cones
- unable to fully determine binding site
- only works for D, not H



[3] Agostino et al., Surf. Sci. **384,** (1997).

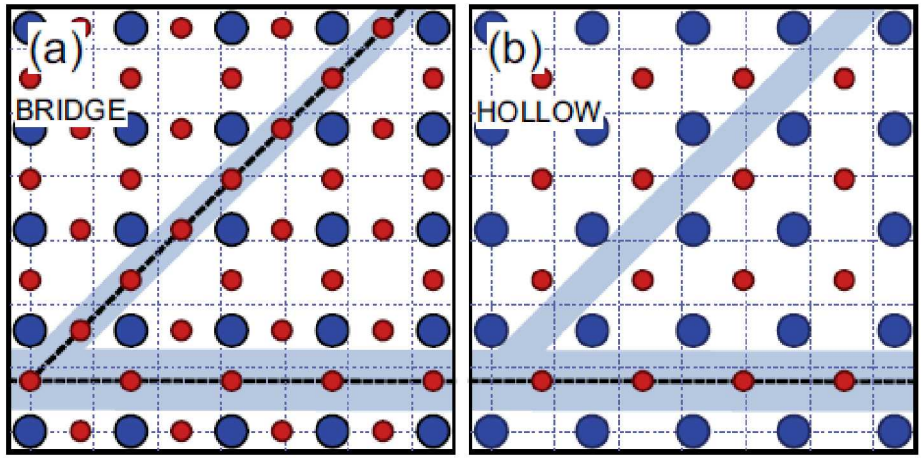
Channeling with multi-angle maps (varying both angles)





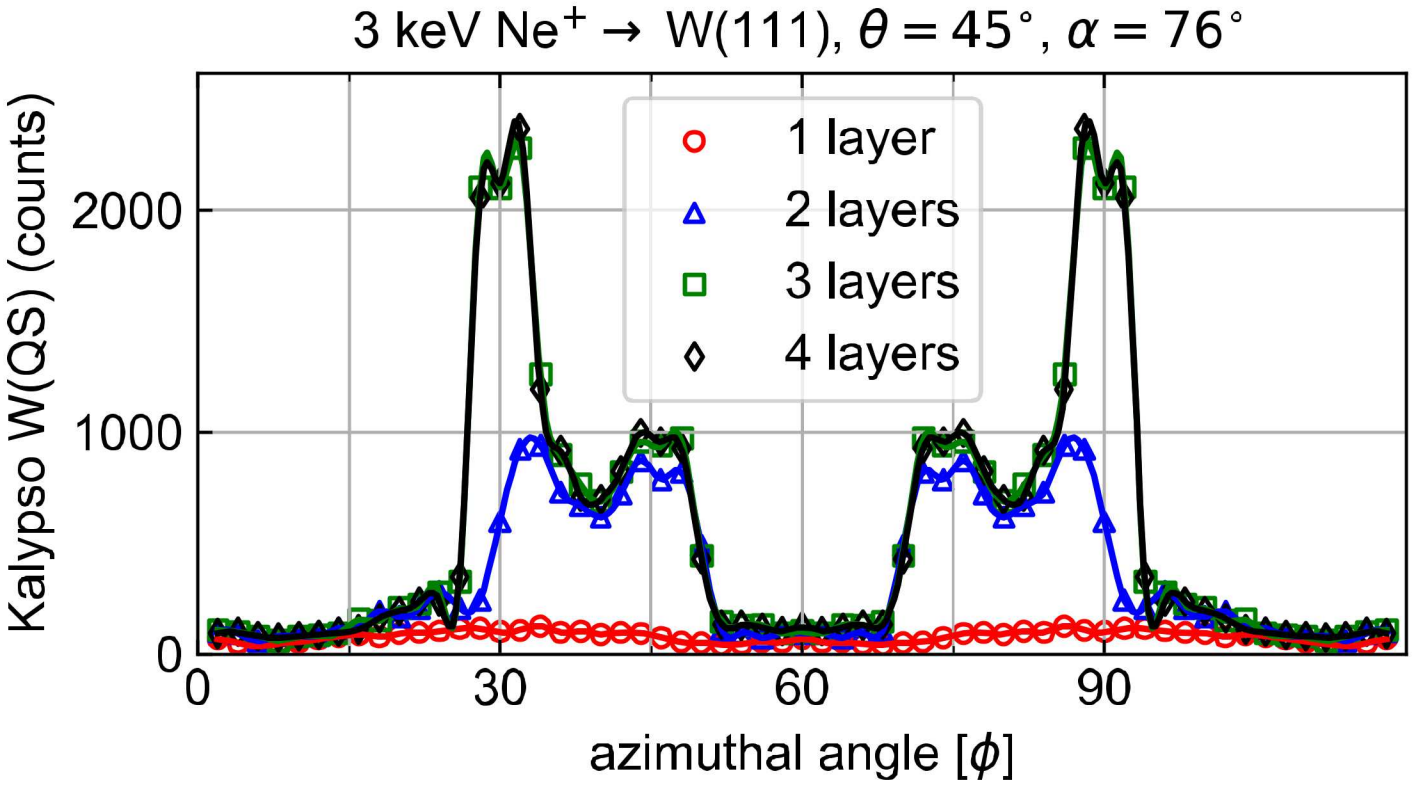
[4] Kolasinski et al., PRB **85,** (2012).

H within channel ➔ recoil peak

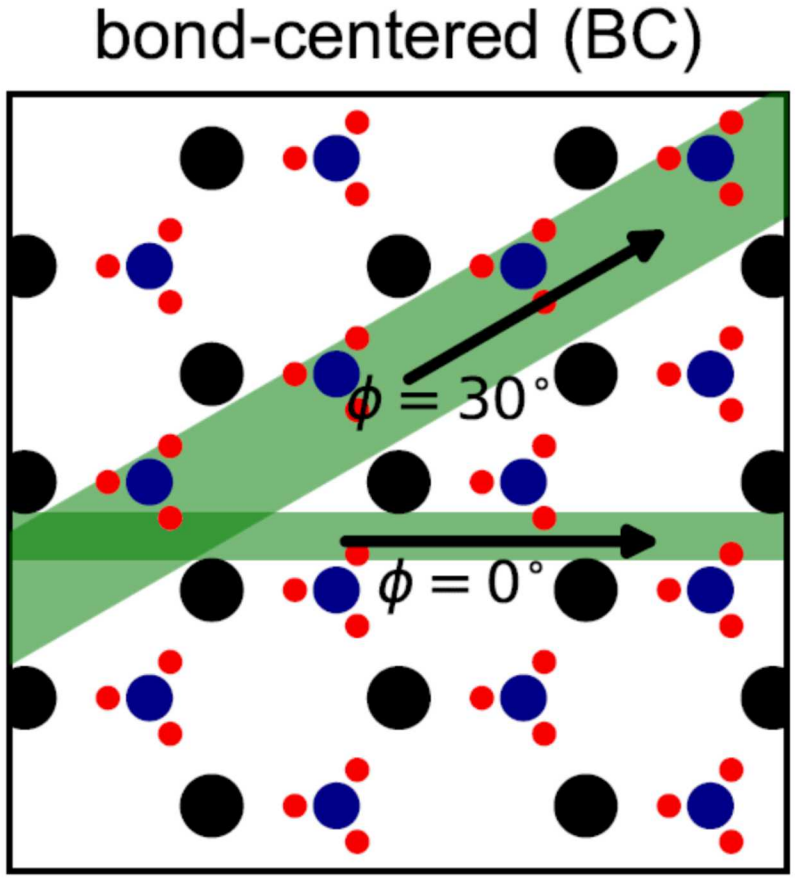


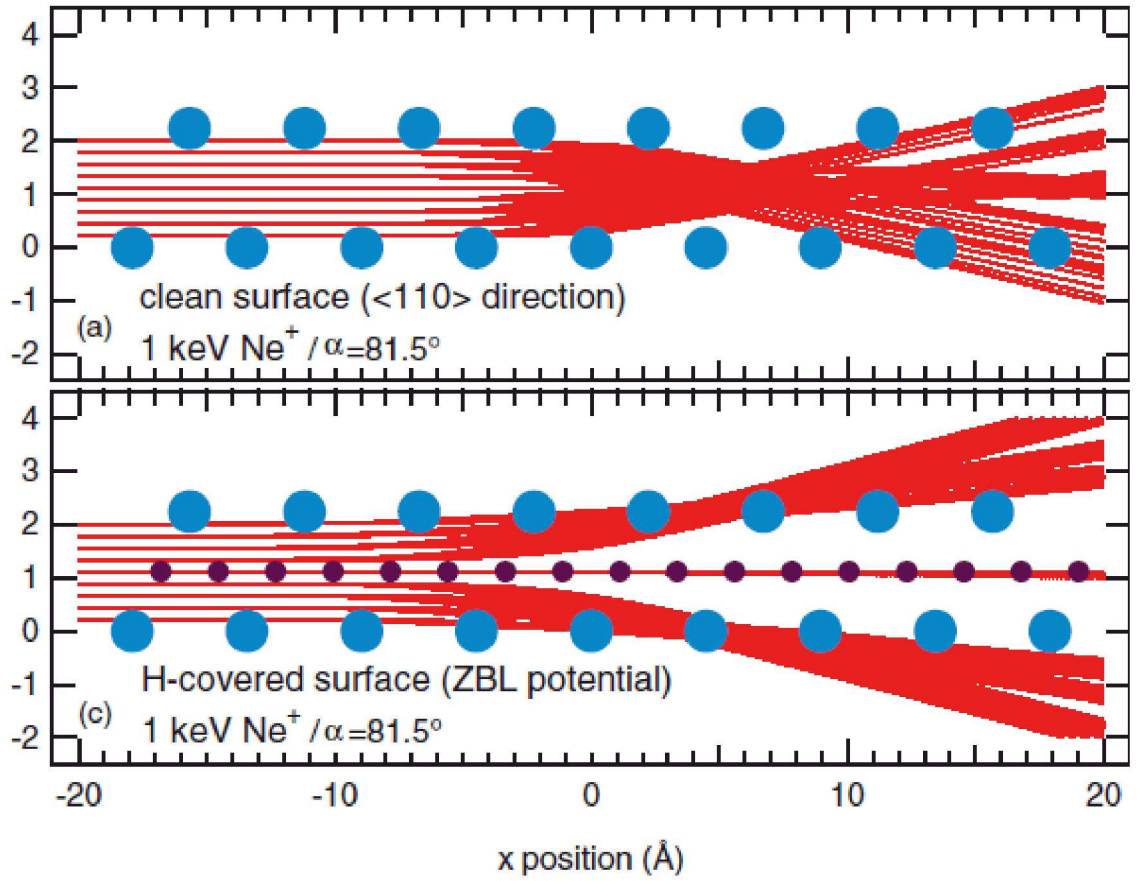
- maps provide information on ion channeling
- detection of adsorbates not limited to near-surface
- only considers scattering from top monolayer and adsorbates
- does not identify complex binding geometries

MD simulation for multi-layer scattering



Effect of hydrogen on ion-channeling

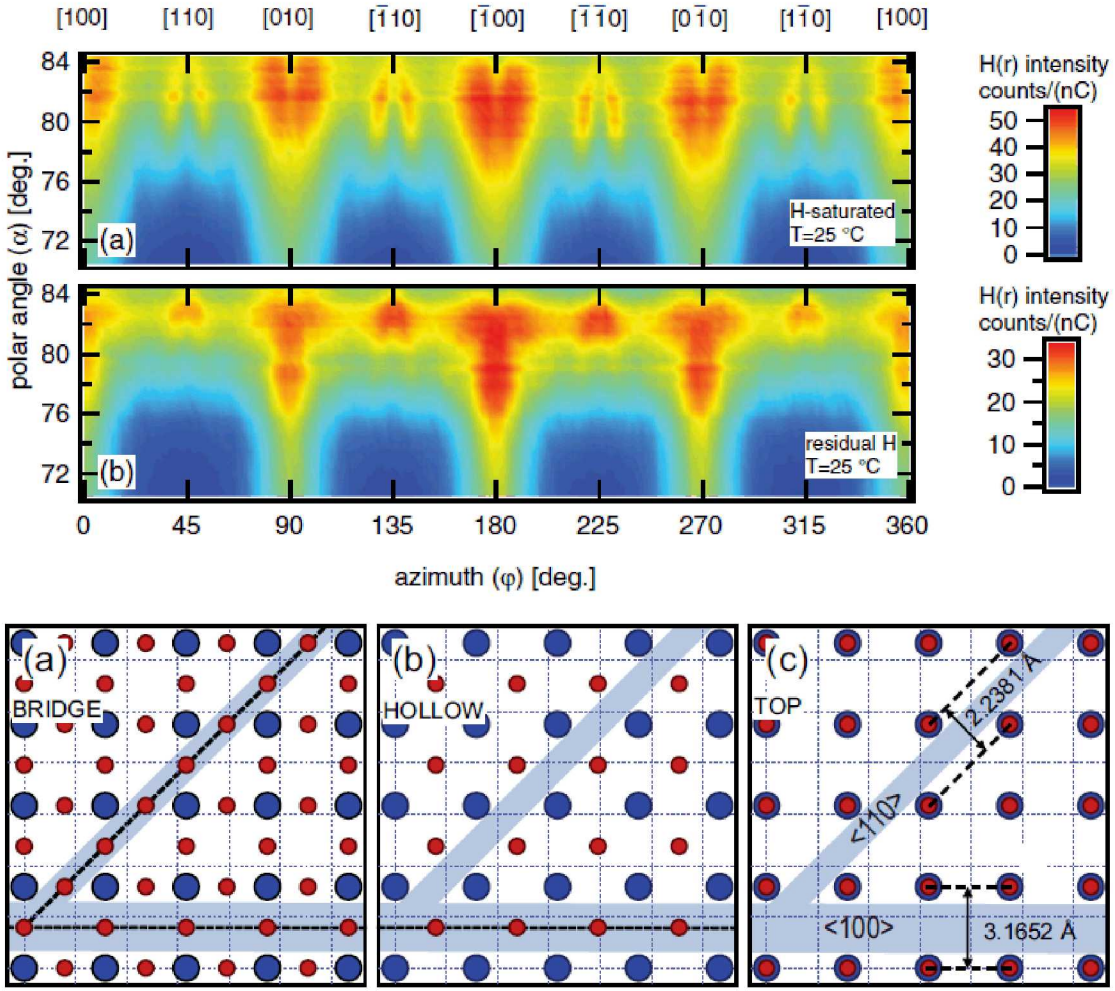


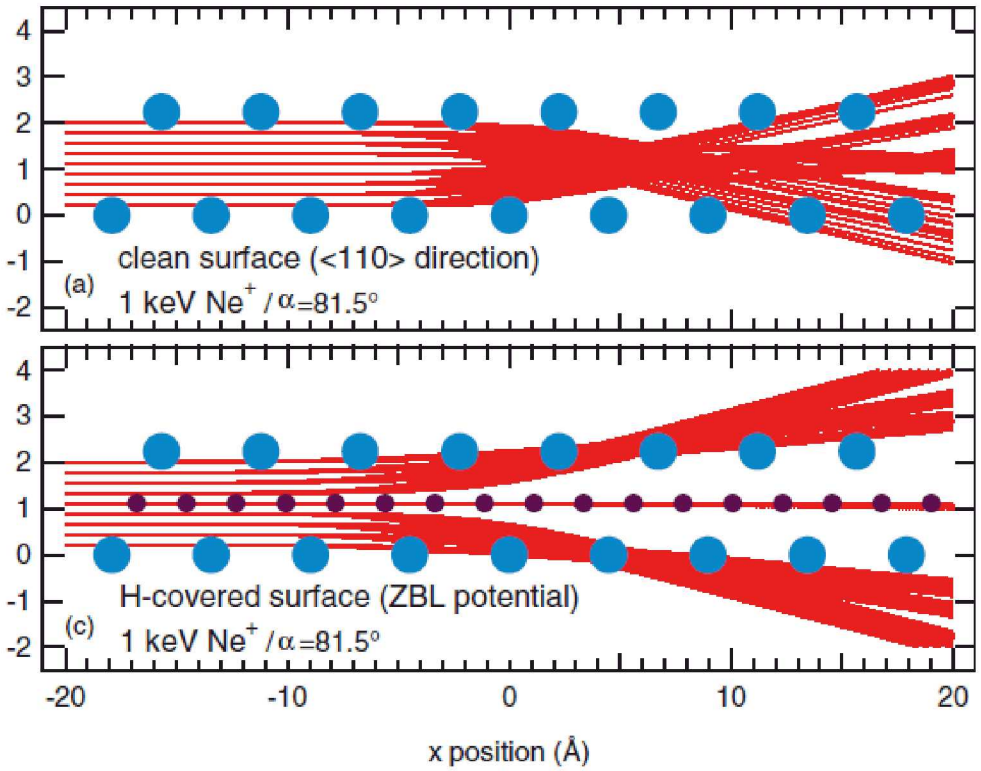


[1] Kolasinski et al., PRB 2012.

State of the art: dechanneling of projectile ions

Surface channeling in W(100)





[1] Kolasinski et al., PRB 2012.