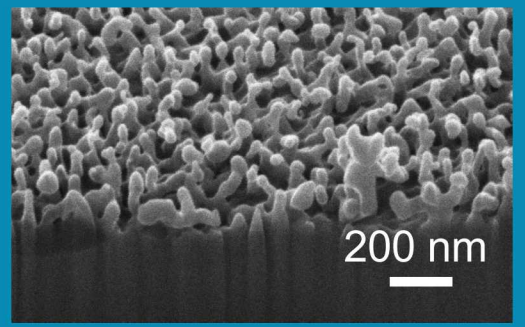
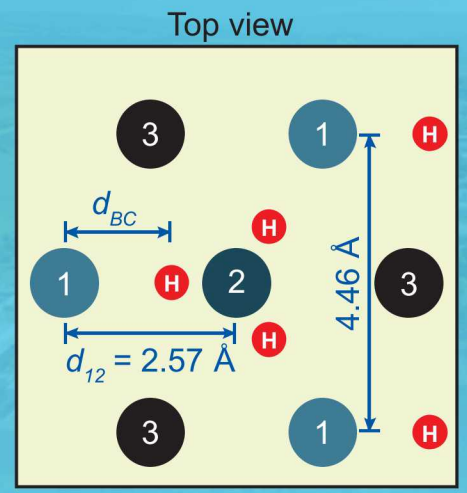
SAND2019-12709C

Helium and hydrogen interactions with tungsten surfaces





PRESENTED BY

Tim Wong | October 23, 2019

Josh A. Whaley and Robert D. Kolasinski

Energy Innovation Department

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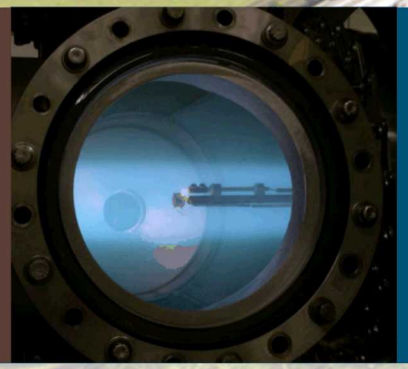
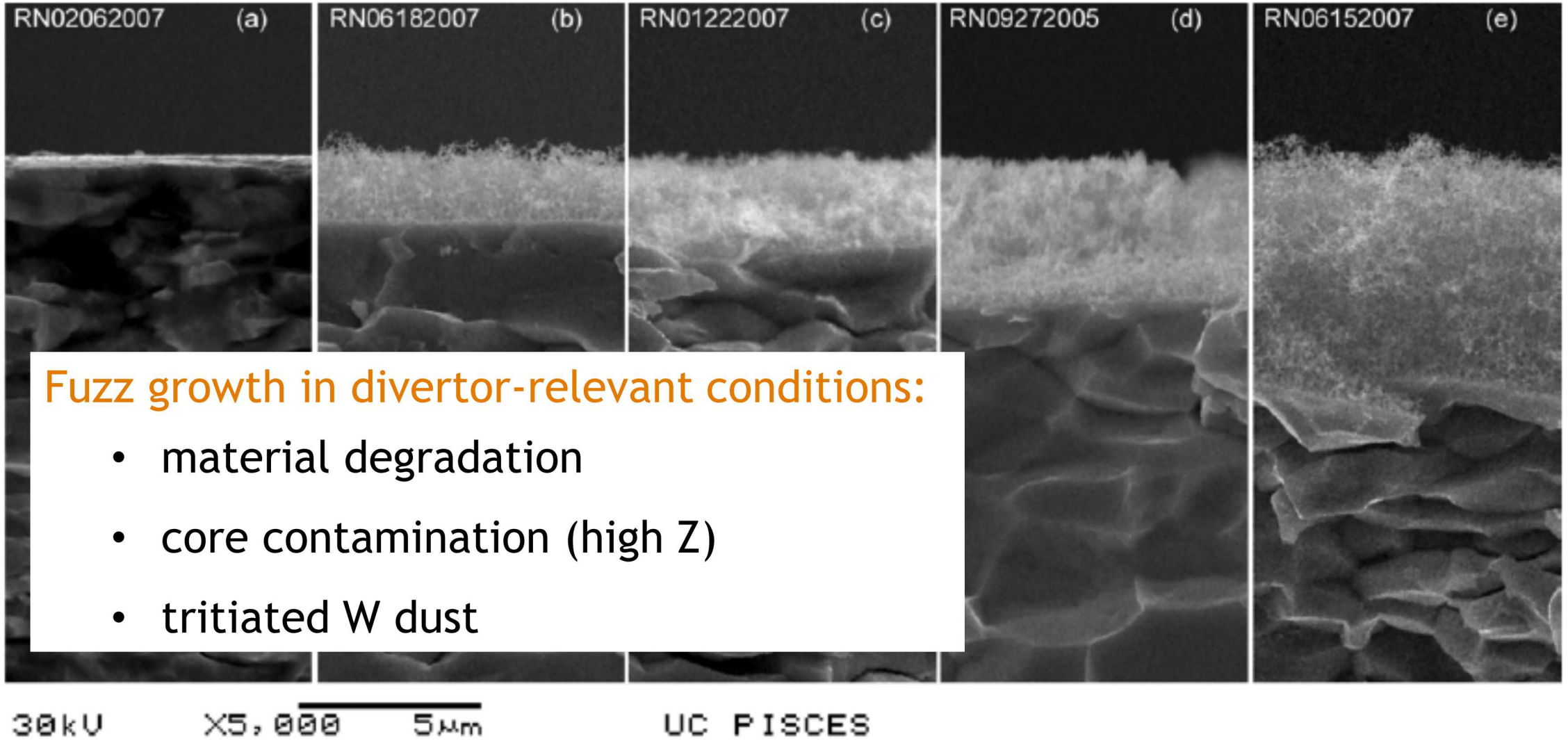


He plasma interactions with W surfaces

Effect of TDS on He-induced W nanostructure

Helium-induced "fuzz" on W surfaces

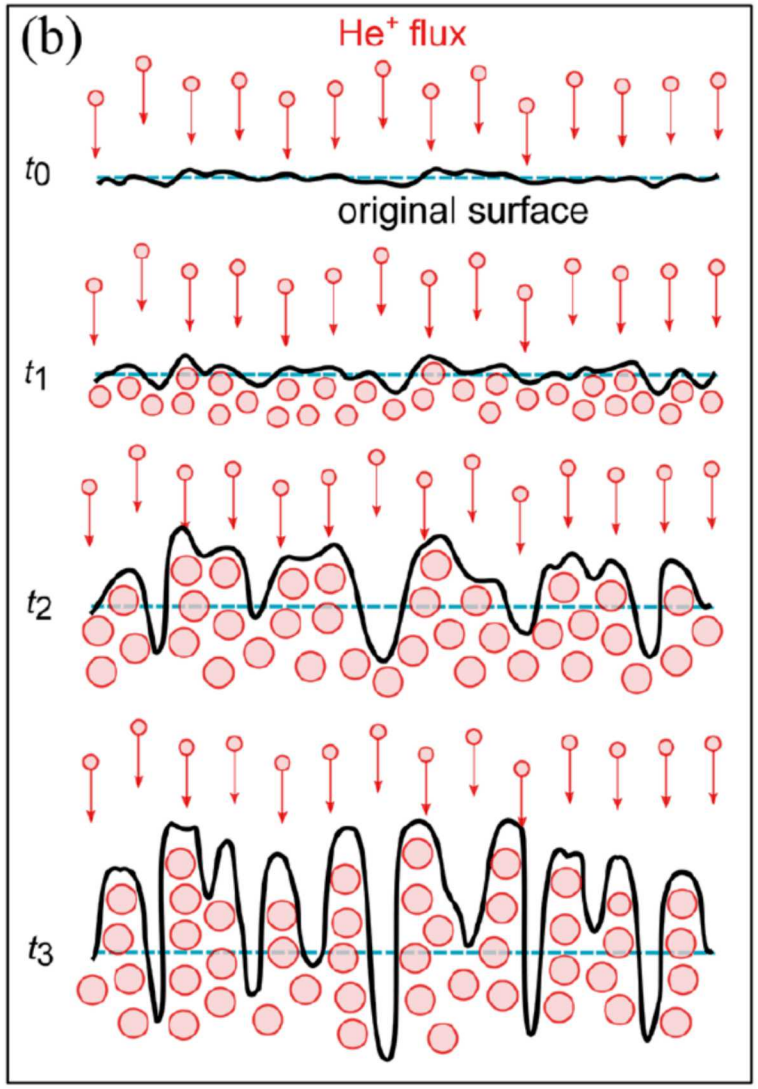


Fuzz growth in divertor-relevant conditions:

- material degradation
- core contamination (high Z)
- tritiated W dust

M.J. Baldwin and R.P. Doerner, Nucl. Fusion (2008).

He-induced nanostructure growth on W surfaces



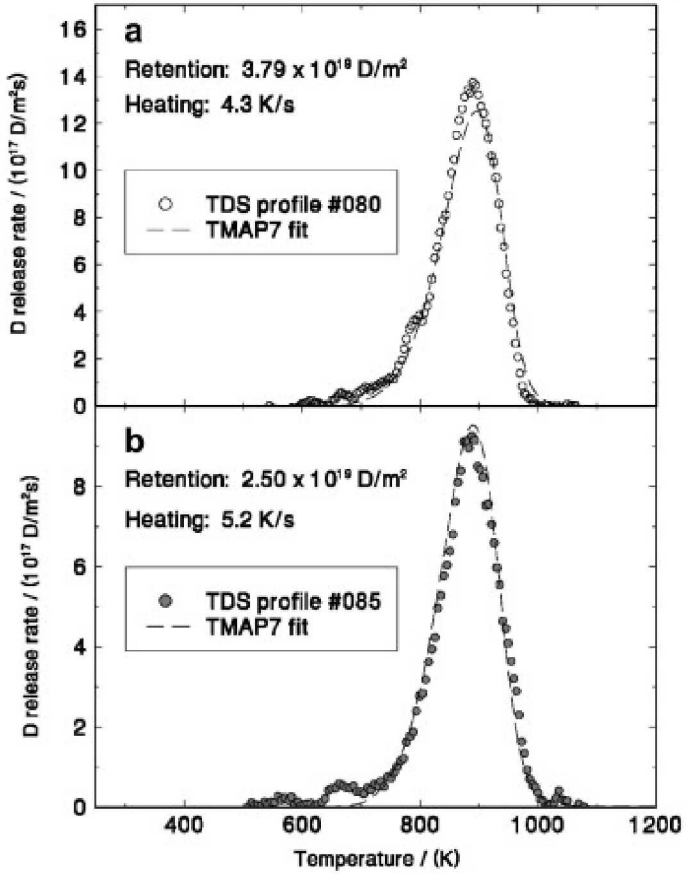
Dasgupta et al., Nucl. Fusion (2019).

- physics for fuzz growth still not well understood
- general steps:
  1. He implanted into W
  2. forms stable pairs of He
  3. coalesce into He bubbles
  4. He bubbles + surface stresses + W adatom diffusion ➔ nanostructure

thermal desorption spectroscopy (TDS) can investigate He-W interactions and trapping

TDS to investigate trapping energies

TDS has been successfully used to determine D binding energies in W

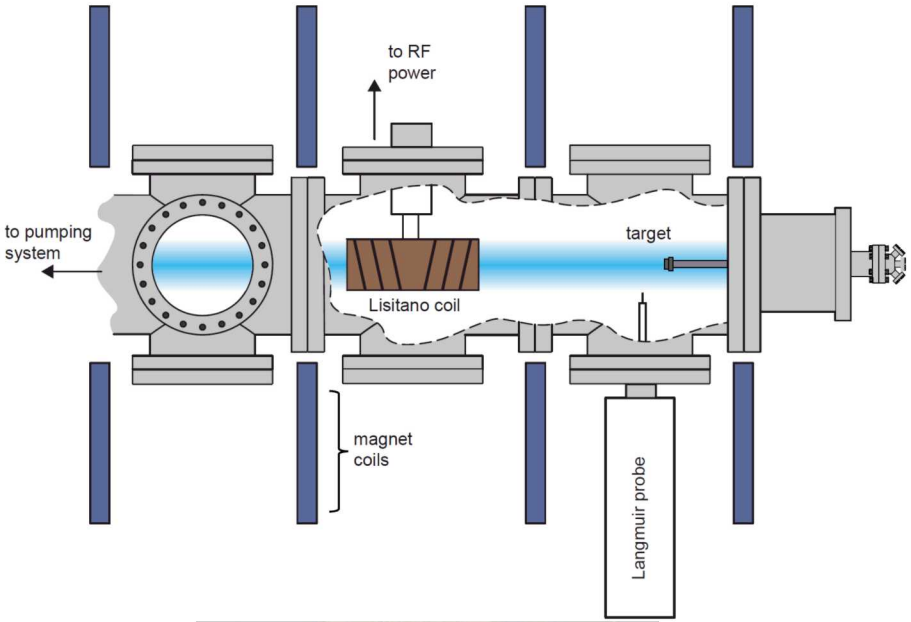


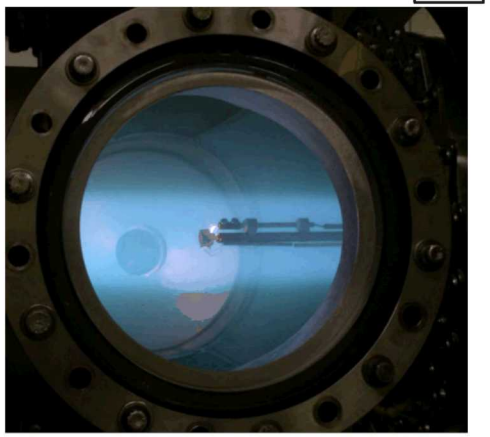
Poon, Haasz, and Davis, J. Nucl. Mater., (2008).

1. Can TDS modeling be done in the same way for He-exposed W?

2. What happens to the nanostructure during TDS (>1800 K needed to fully desorb He)?

Plasma exposure and conditions





W sample exposed to He plasma

Plasma conditions

ion flux	Γ_{ion}	= 4.0 × 10^{16} cm^{-2} s^{-1}
electron temp.	T_e	= 11 eV
plasma potential	V_p	= 40 V
plasma density	n_p	= 2.0 × 10^{10} cm^{-3}

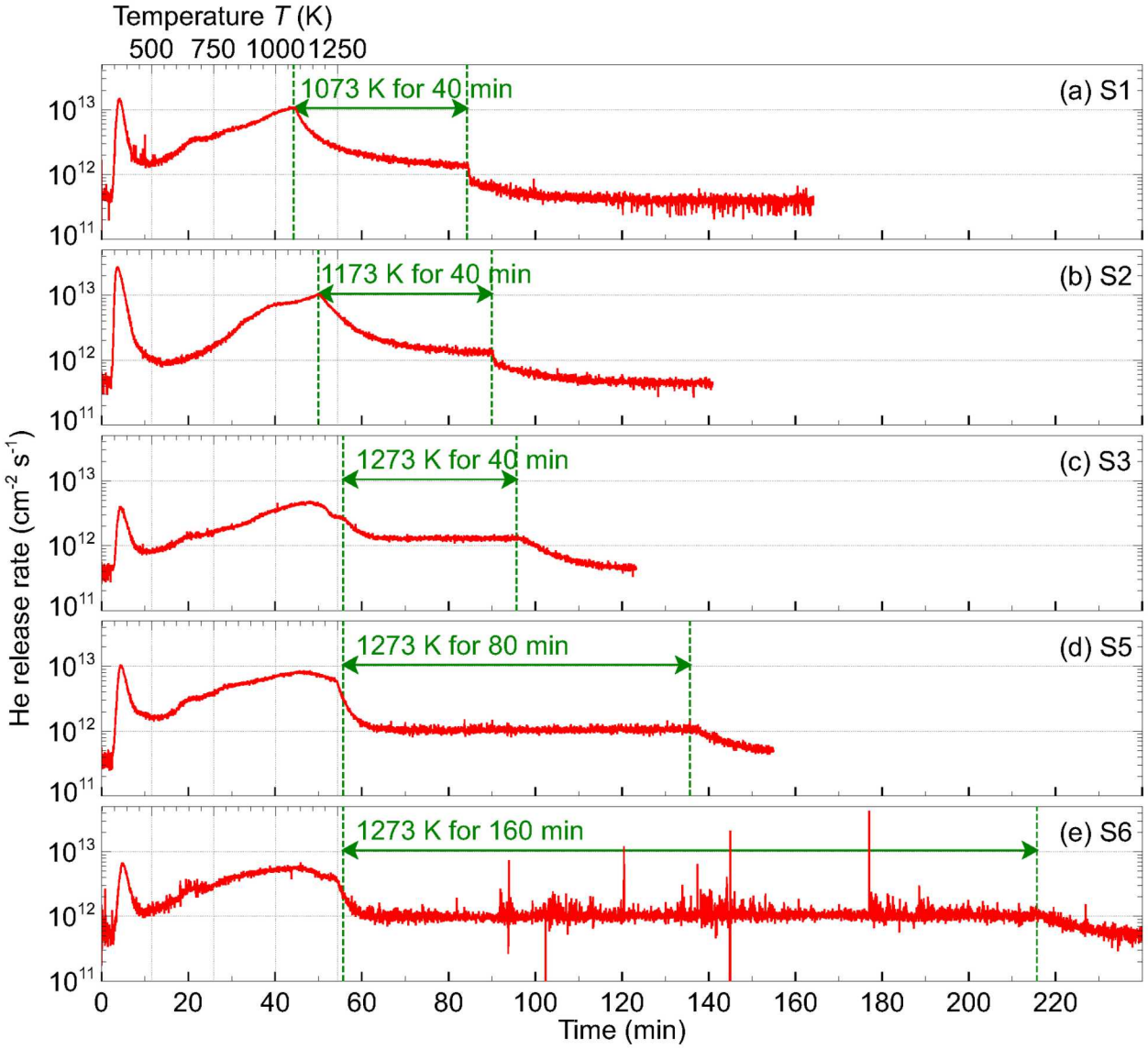
Plasma exposure (same for all samples):

(1) 6 hours in plasma

(2) held at 1123 K

(3) biased at -50 V (ion energy of 90 V)

Thermal desorption spectroscopy



- consistent desorption peaks near T=373 K and 1123 K for all samples
- 1123 K peak observed in literature for similar He-plasma exposures
- spikes in (e) are indication of bursting of near-surface He bubbles

Ramp rate of 17.5 K s^{-1}

Post-TDS surface characterization

Helium ion microscopy

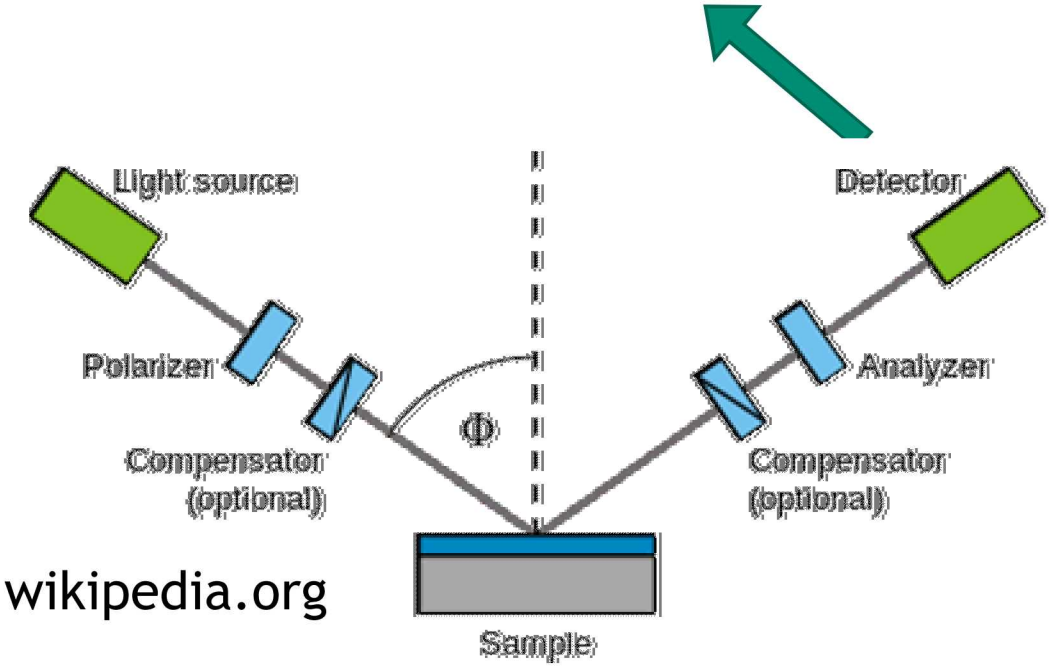
- better depth of field, resolution, and contrast than SEM (but $$)
- performed at UC Berkeley BNC

zeiss.com

Spectroscopic ellipsometry

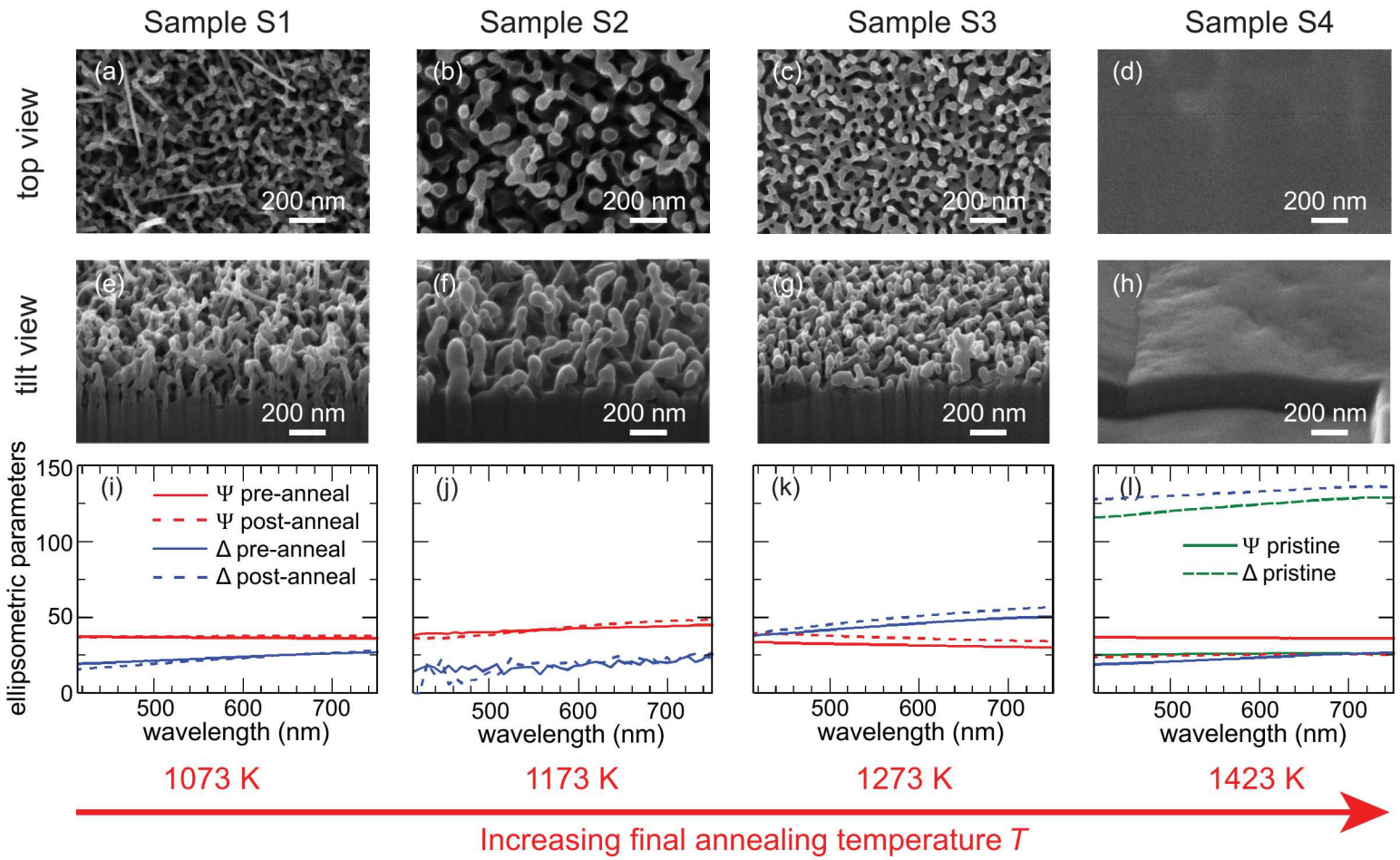
- can be performed in-situ and in real time
- non-destructive & contactless
- sensitivity to nm-sized changes

Ellipsometric parameters: Ψ, Δ



wikipedia.org

Effect of annealing temperature on surface morphology

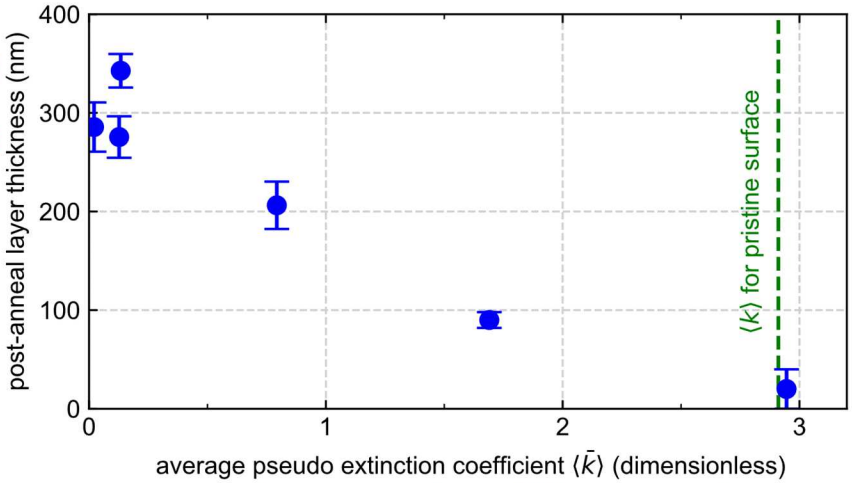


held at *T* for 40 min

changes to nanostructure starting around 1173 K

fully recrystallized at 1423 K

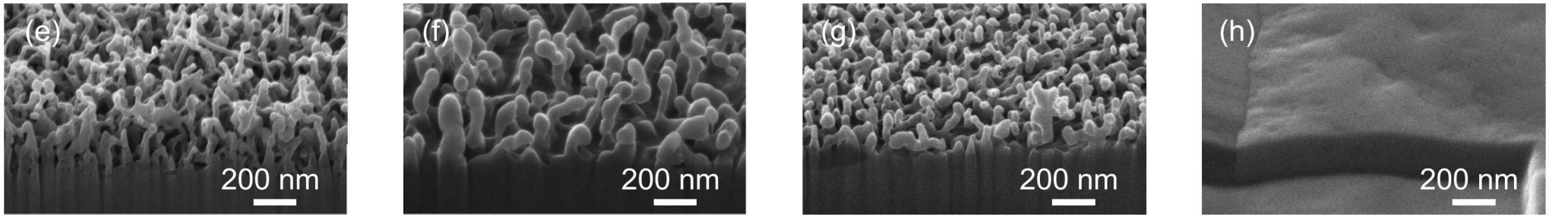
HIM imaging

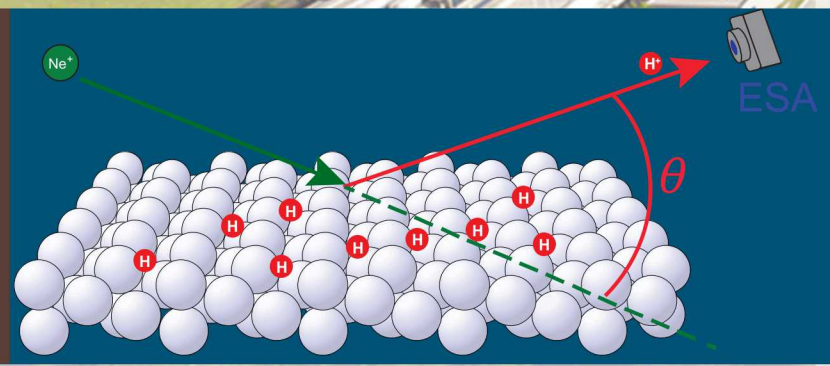


spectroscopic ellipsometry

Conclusions for high-temperature annealing study

1. TDS can greatly alter surface morphology of W nanostructure
   - changes observed at 1173 K
   - full recrystallization at 1423 K after 40 min
2. modeling of TDS spectra should account for complications that may arise from changing surface morphology
3. ellipsometry can potentially be used to track surface recovery in-situ





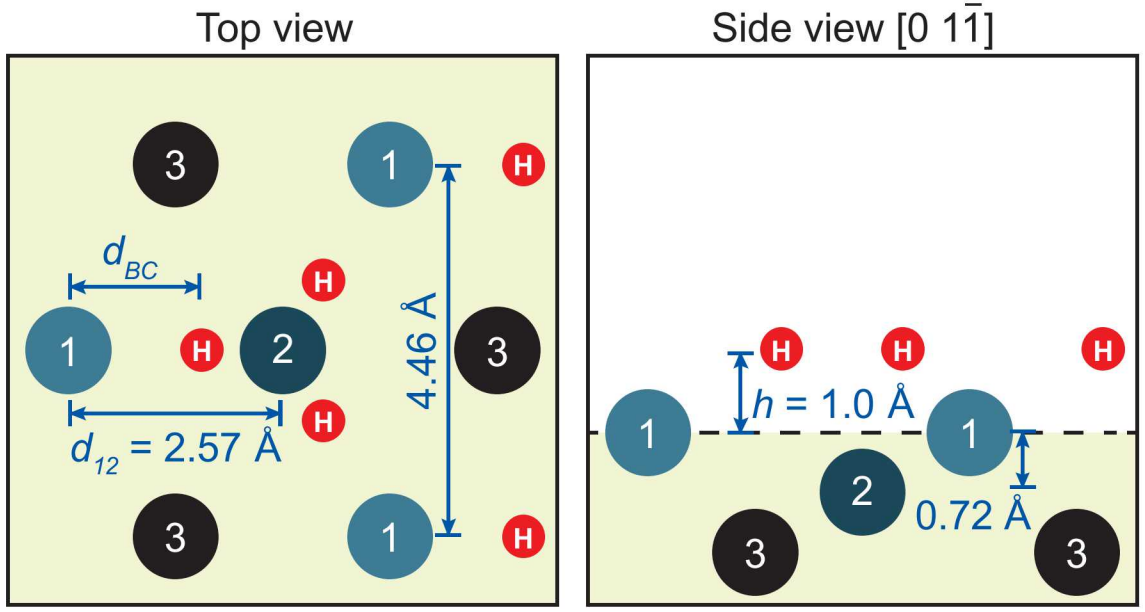
Hydrogen adsorption on W surfaces

Characterizing the W(111)+H(ads) system

DFT predictions of H adsorption on W(111)

Bond-centered (BC) H adsorption on W(111) was predicted using DFT [1]

by Z. Bergstrom, Brian Wirth's group at U. Tennessee



1.49 Å ≤ d_{BC} ≤ 1.69 Å 0.96 Å ≤ h ≤ 1.12 Å

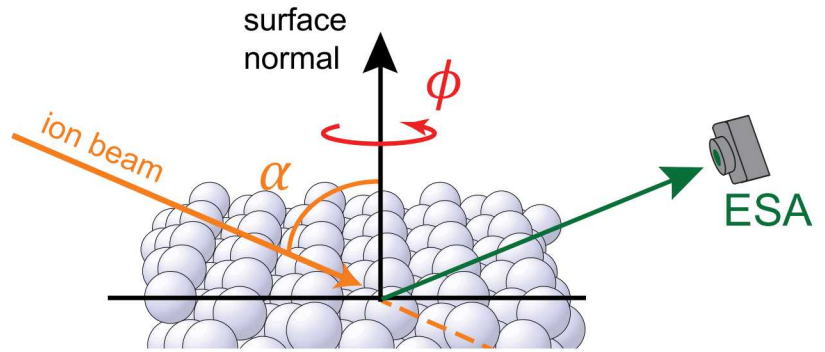
Experimentally validate DFT results:

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

- interparticle potentials for MD
- hydrogen dissociation energies on surfaces

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

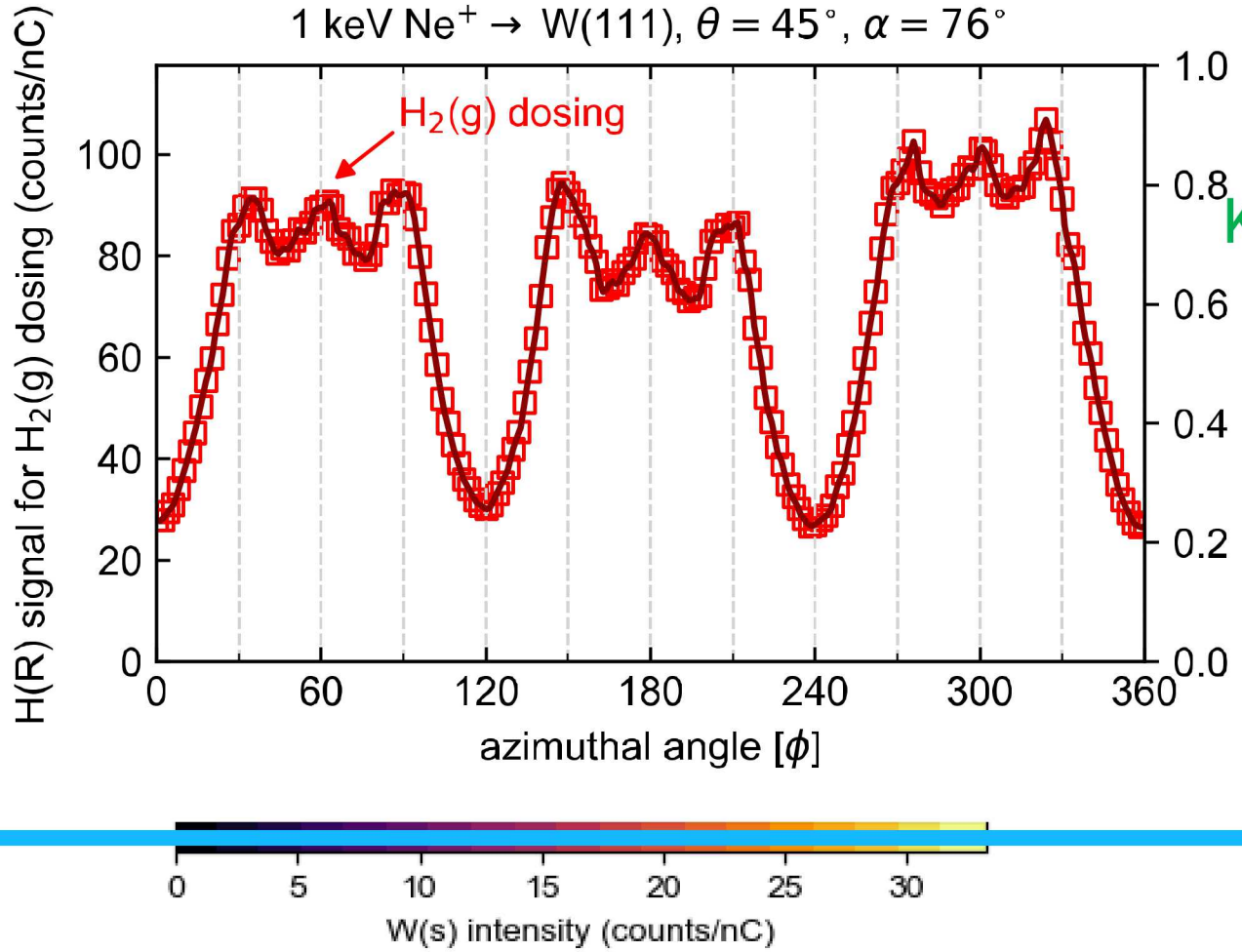
Low energy ion scattering (LEIS)



Model this signal with MD to identify H binding sites

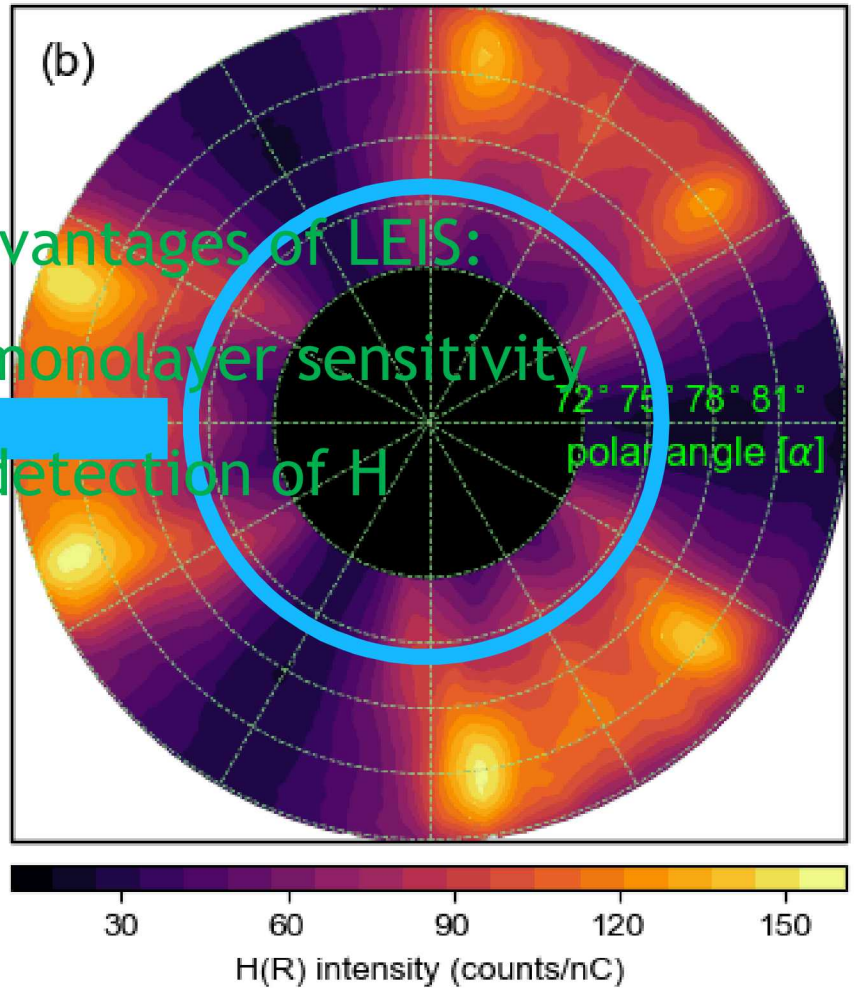
Scattering signal from W substrate

Recoil signal of H from ion channeling

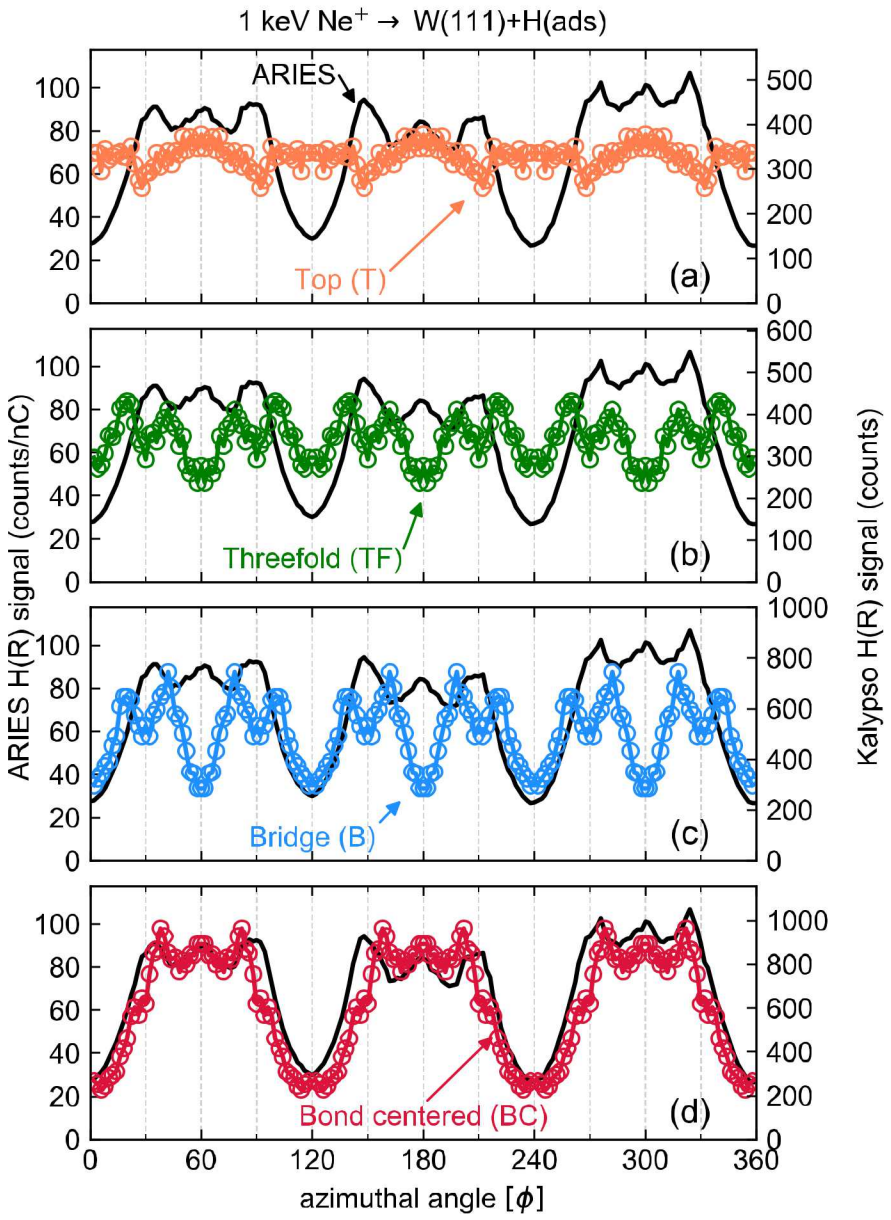


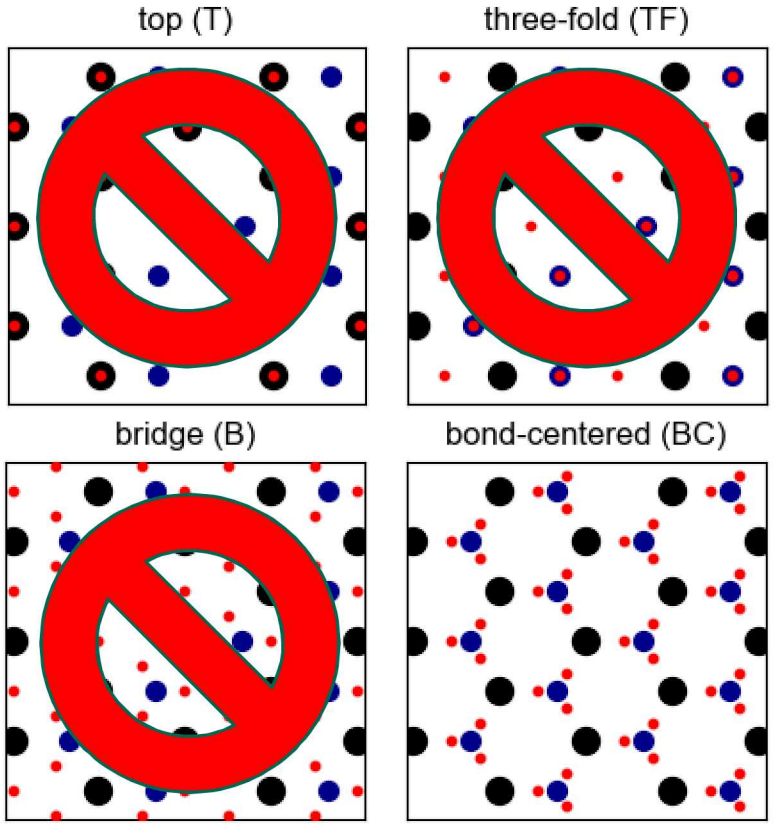
Key advantages of LEIS:

- monolayer sensitivity
- detection of H



Experimental data compared to MD simulation (Kalypso [2])





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

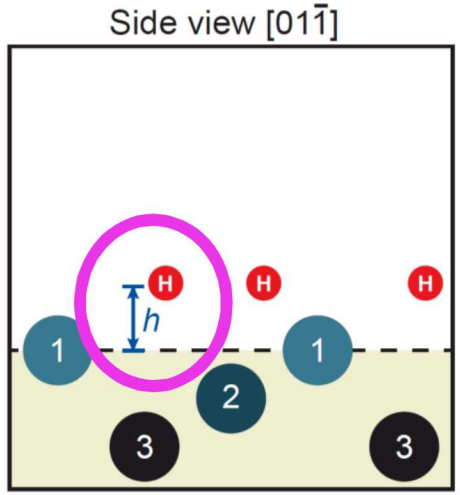
Constraining adsorbate height and position

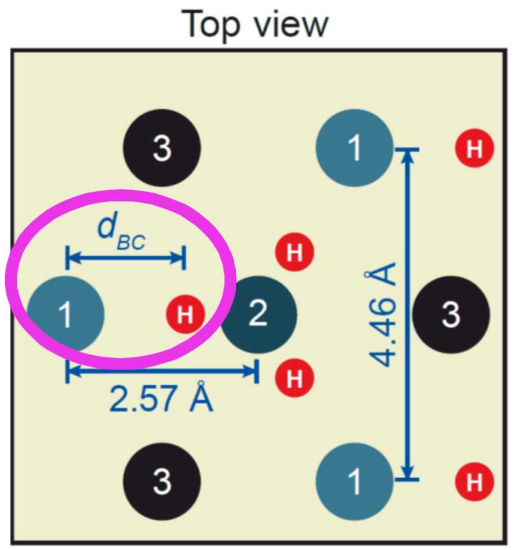
h = 1.0 ± 0.1 Å

DFT prediction:
0.96 Å ≤ h ≤ 1.12 Å

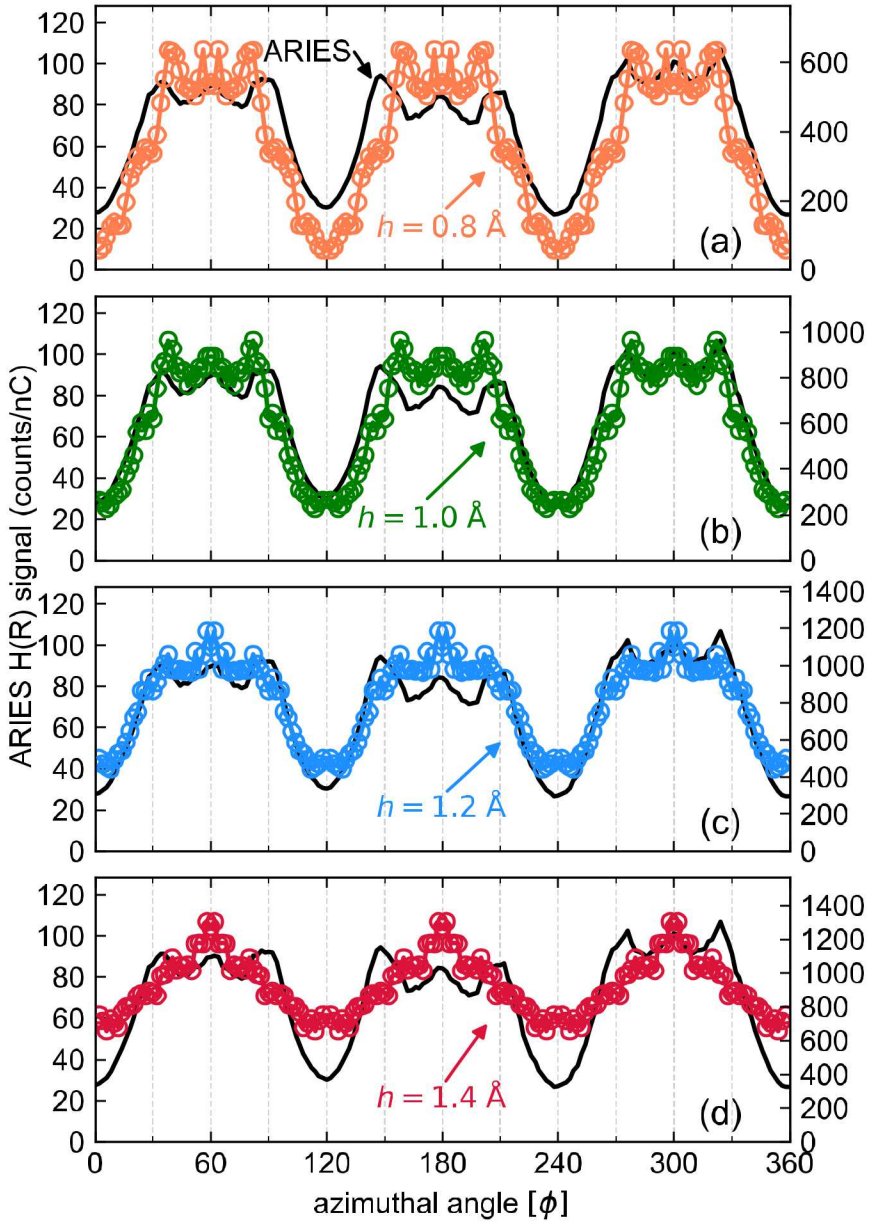
d_{BC} = 1.6 ± 0.1 Å

DFT prediction:
1.49 Å ≤ d_{BC} ≤ 1.69 Å



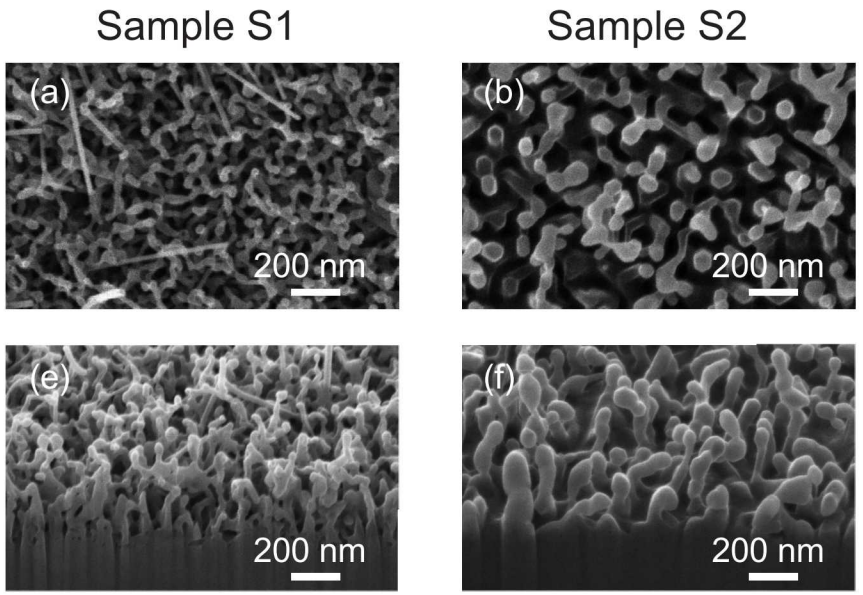


varying h

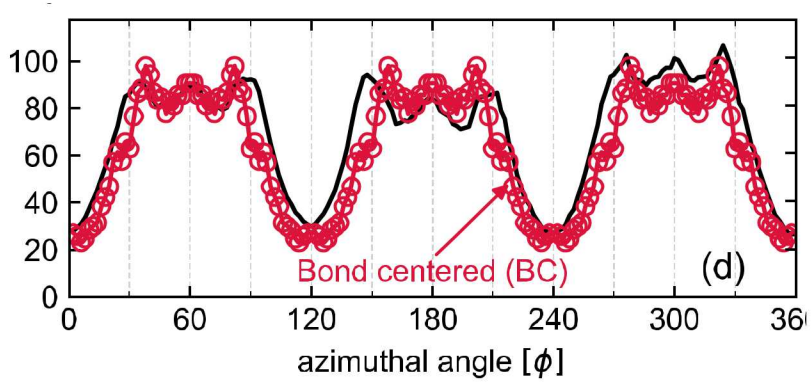


Summary

1. TDS of He-induced W nanostructure
   - changes in morphology observed at 1173 K (≪1800 K for full He desorption)
   - interpretation of TDS data needs to account for changes in surface nanostructure



2. Validated bond-centered (BC) hydrogen binding for the W(111)+H(ads) system

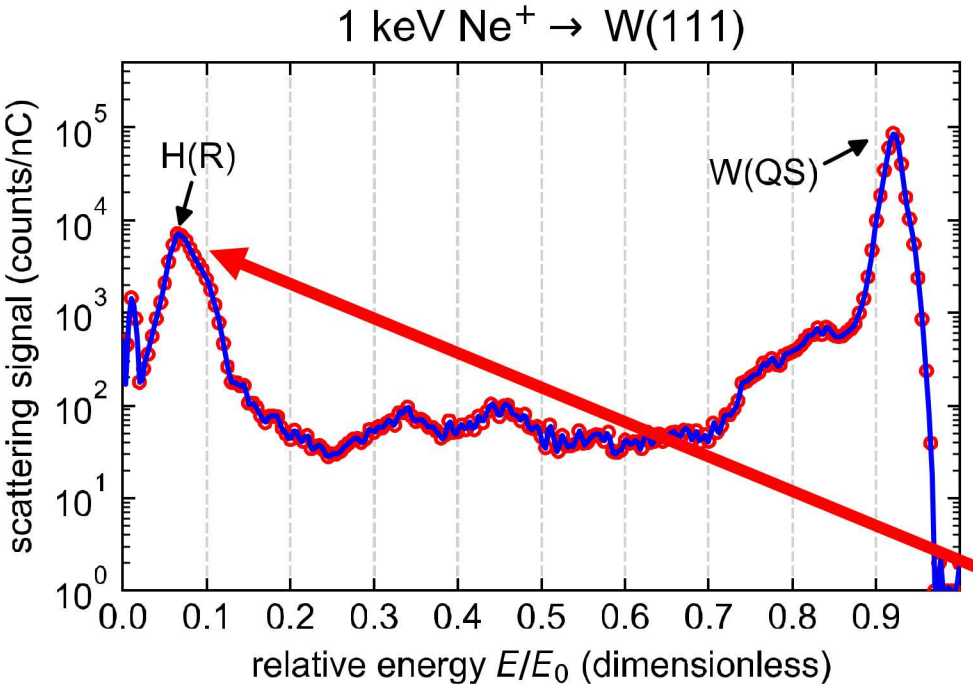


Thank you for your attention!

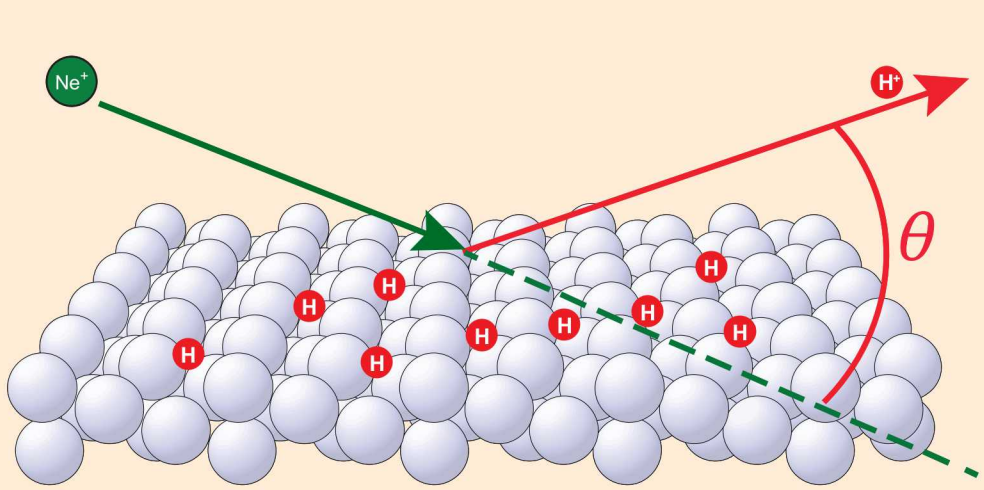
Extra slides

Direct recoil spectroscopy

One of the few surface science techniques with hydrogen sensitivity

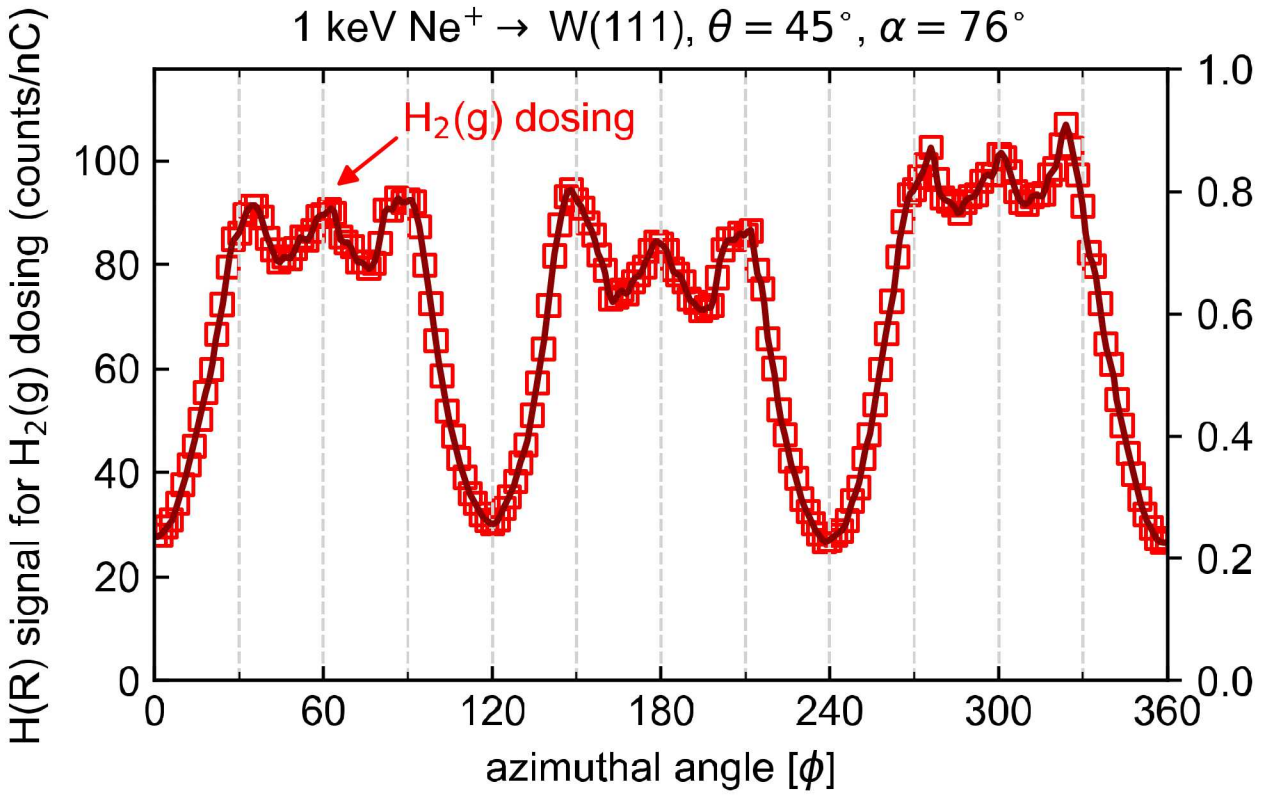


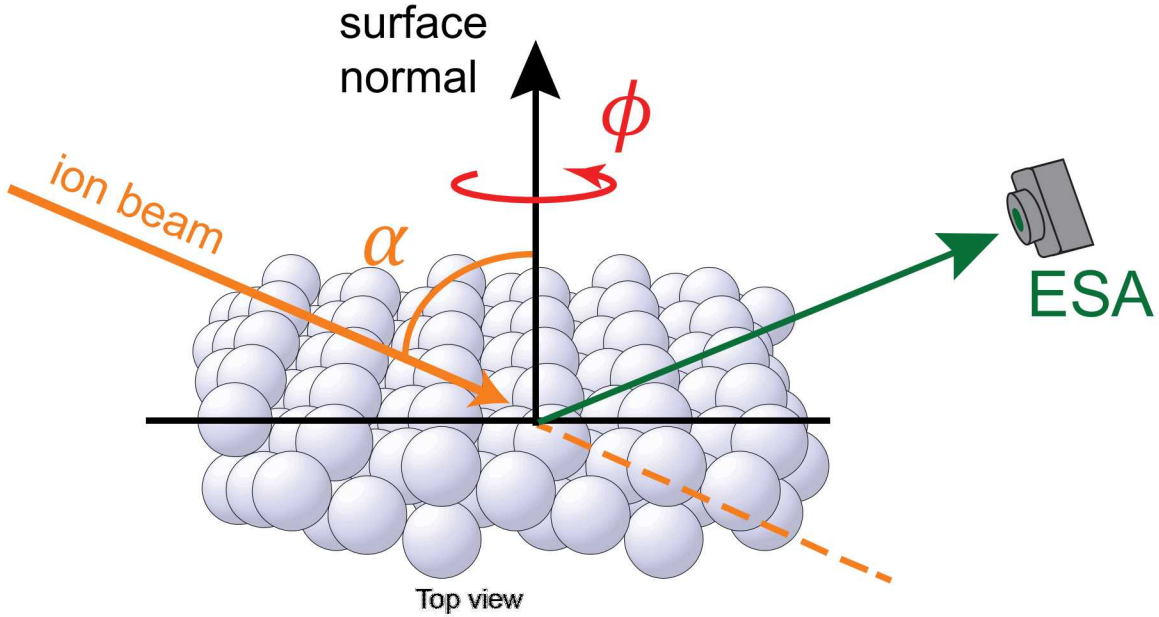
Direct recoil spectroscopy (DRS)

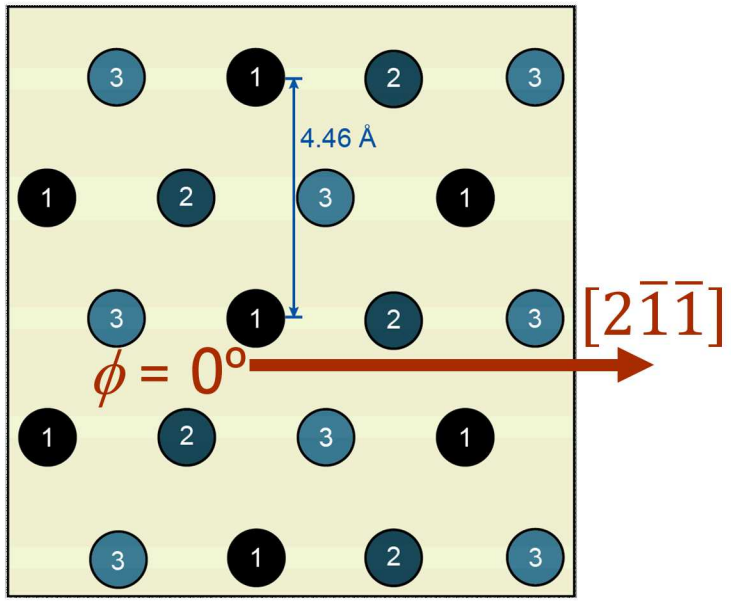


$$\frac{E}{E_0} = \frac{4\mu}{(1+\mu)^2}\cos^2\theta\,, \quad \mu = \frac{m_T}{m_P}$$

Obtaining H recoil measurement at a single α

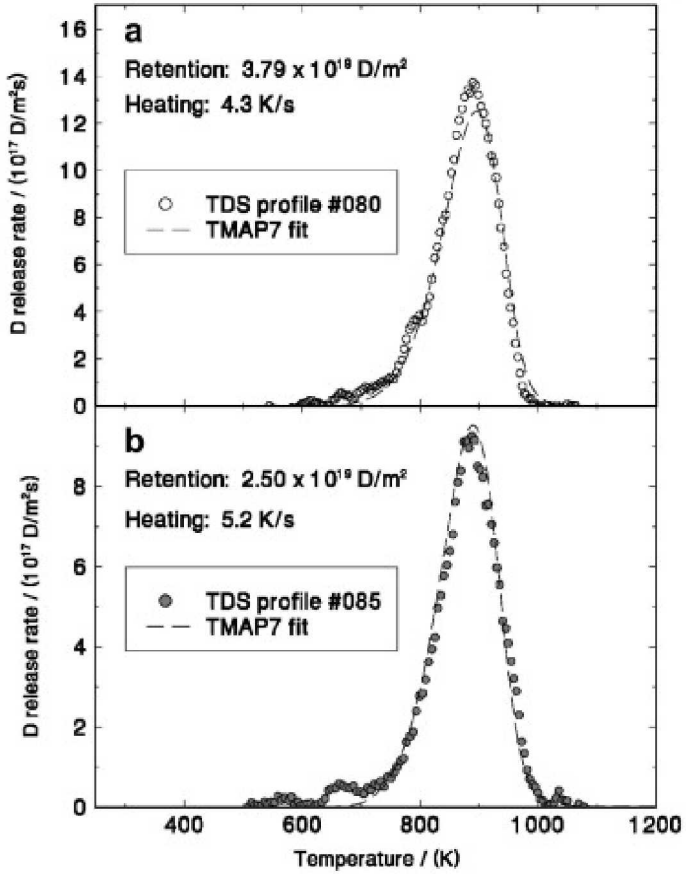






TDS to investigate trapping energies

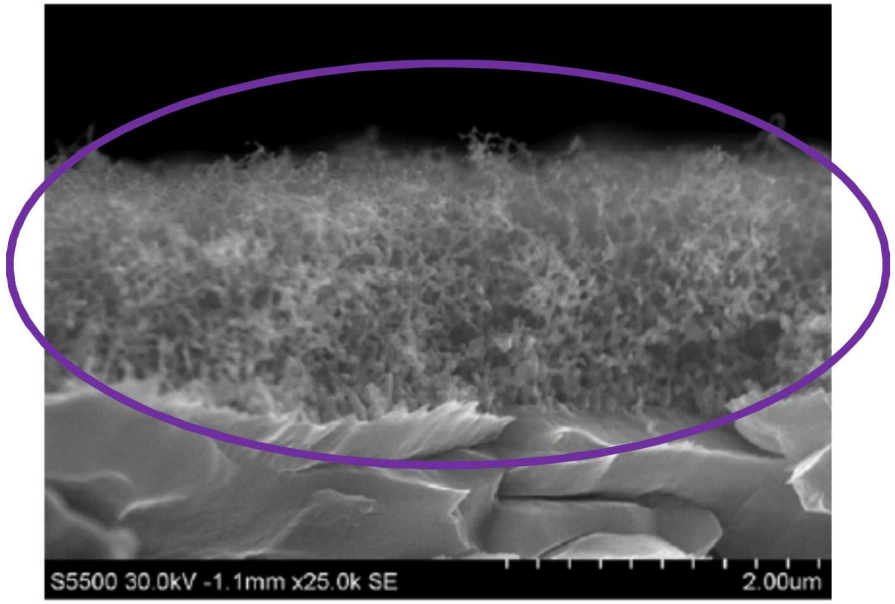
TDS has been successfully used to determine D binding energies in W



Poon, Haasz, and Davis, J. Nucl. Mater., (2008).

1. Can TDS modeling be done in the same way for He-exposed W?
2. What happens to the nanostructure during TDS (>1800 K needed to fully desorb He)?

up to 60% of retained He found in the fuzz



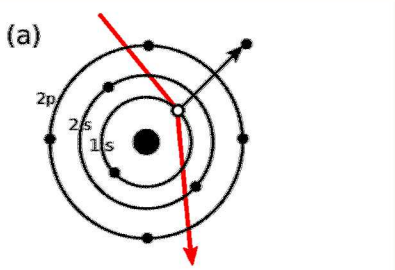
Gasparyan, Efimov, and Bystrov, Nucl. Fusion, (2016).

Detection of surface hydrogen is challenging

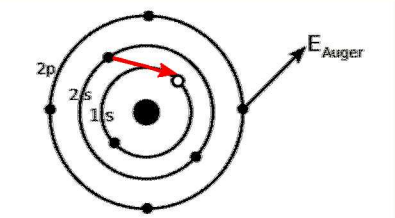
Not many experimental techniques are directly sensitive to surface hydrogen

AES

Auger electron spec.



Electron collision



Auger electron emission

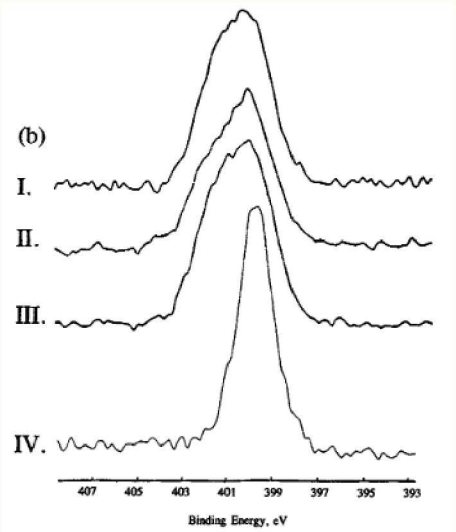
wikipedia.org

no auger electrons for H

XPS

X-ray photoelectron spec.

Shifts in N 1*s* peaks possibly due to H bonding



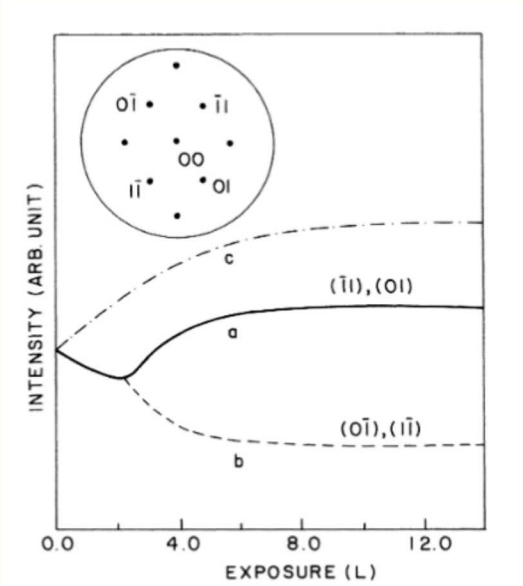
Kerber et al., J. Vacuum Sci. Tech., (1996).

small shifts in peaks due to H binding

LEED

Low energy electron diffraction

Reconstruction of W(110) due to H adsorption



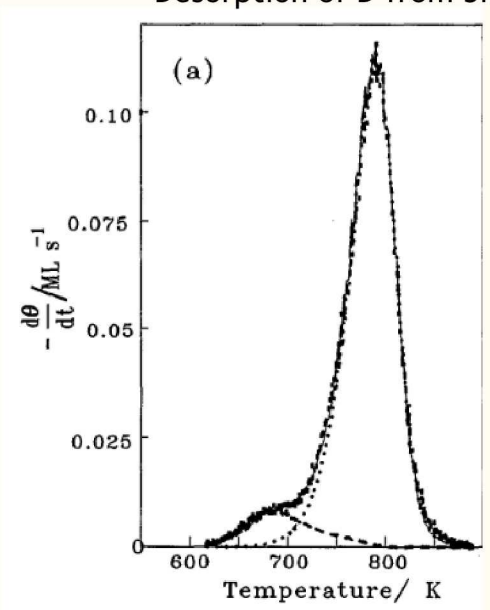
Chung et al., PRL, (1986)

indirect H detection from reconstruction

TPD

Temp. programmed desorption

Desorption of D from Si



Flowers et al., J. Chem. Phys. 1993.

H amount and activation energies, not locations