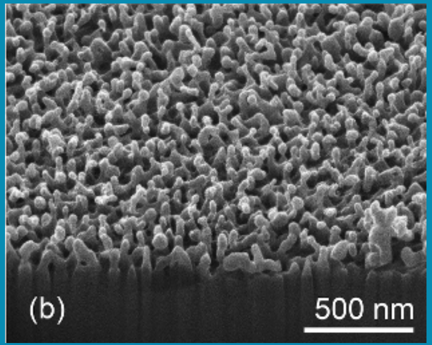
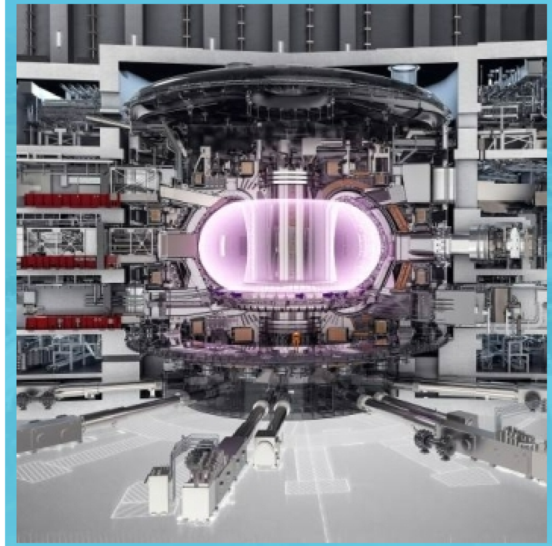
SAND2021-12446PE

Sandia National Laboratories

Materials challenges for magnetic fusion energy





PRESENTED BY

Chun-Shang "Tim" Wong | Oct. 8, 2021

Josh Whaley and Robert Kolasinski

U.S. DEPARTMENT OF ENERGY NNSA

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OAK RIDGE National Laboratory

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Outline

Fusion energy & materials challenges

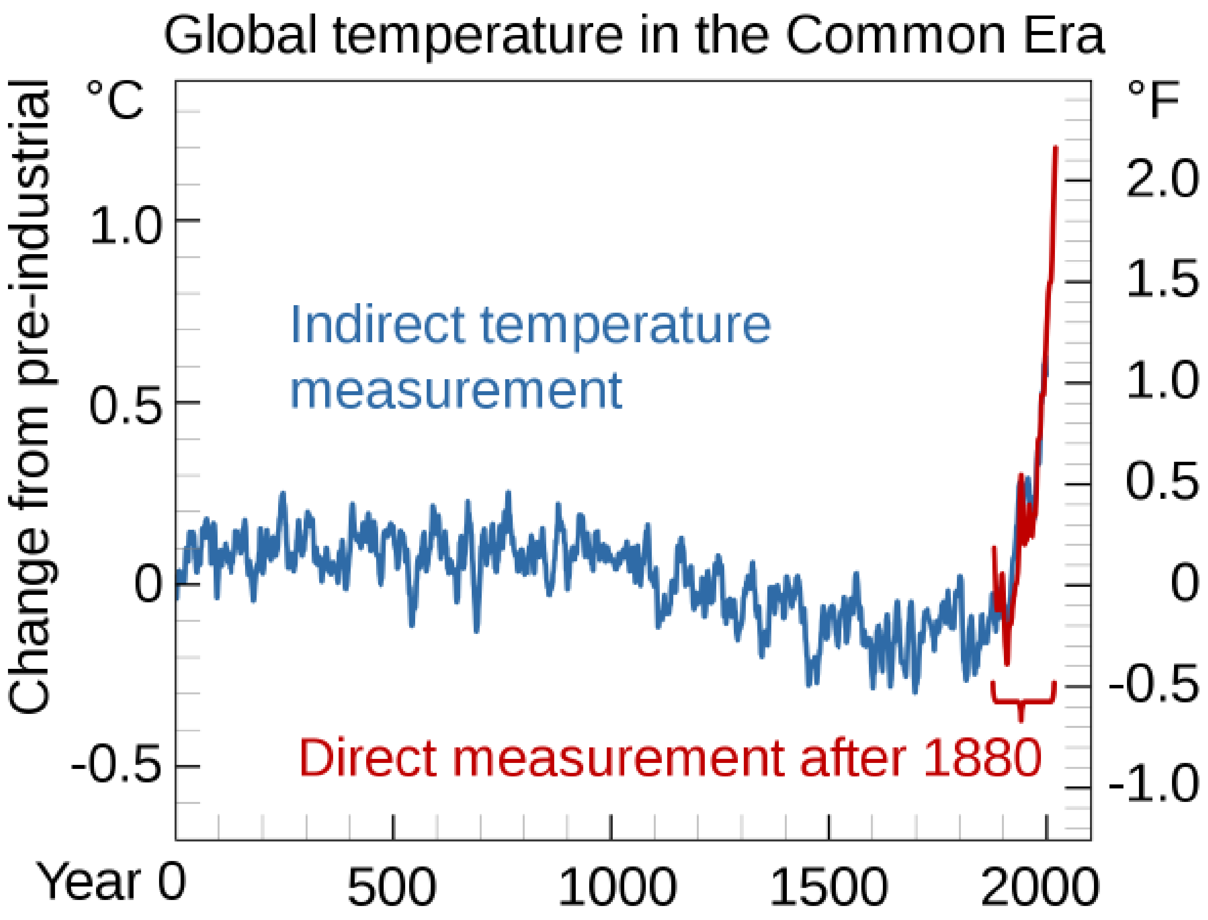
- What is fusion and how does it work?
- What are key materials issues that need to be addressed?

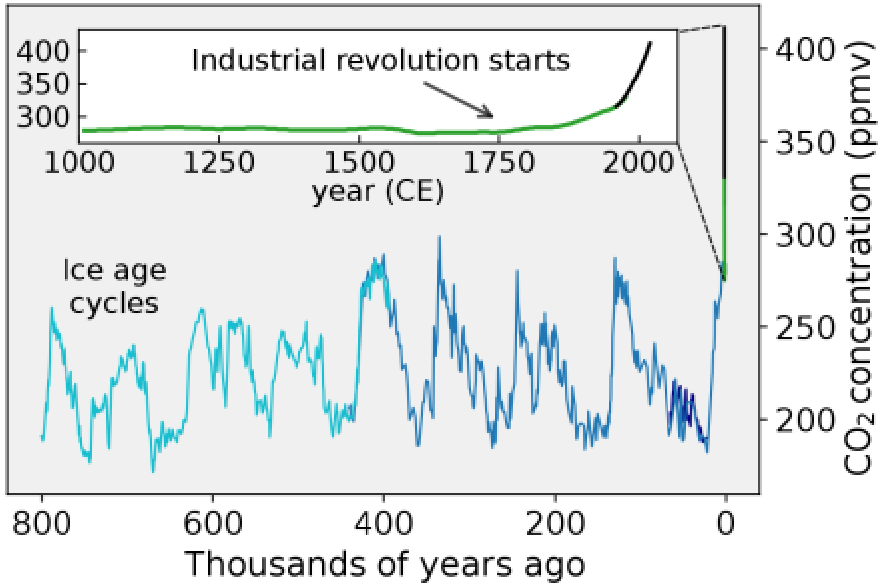
Low energy ion beam analysis of material surfaces

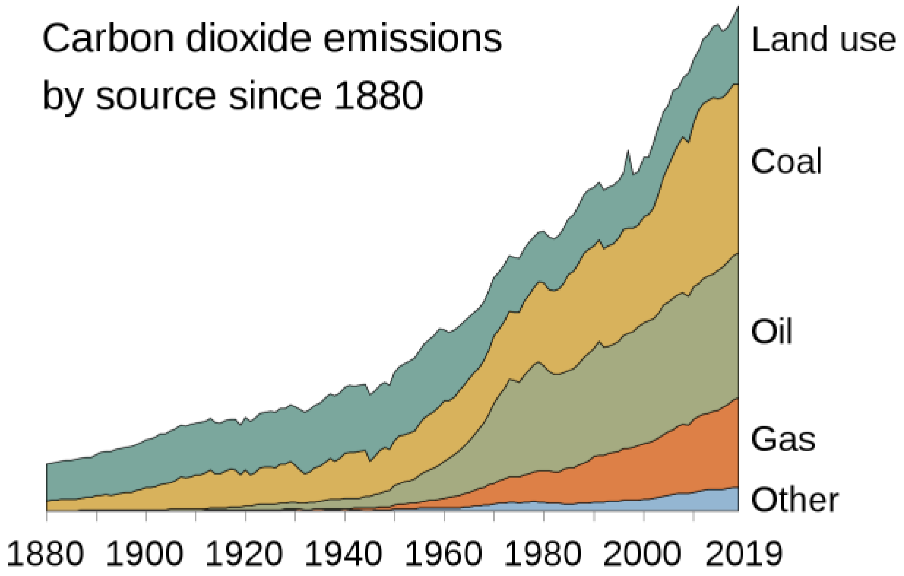
- Hydrogen adsorption on tungsten(111)
- Structural studies of tungsten(111) to understand defect nucleation & growth
- Ongoing/future work
  - Impurity effects on hydrogen adsorption on tungsten surfaces
  - Characterization of more complex surface structures

Summary

Climate change due to reliance on fossil fuel

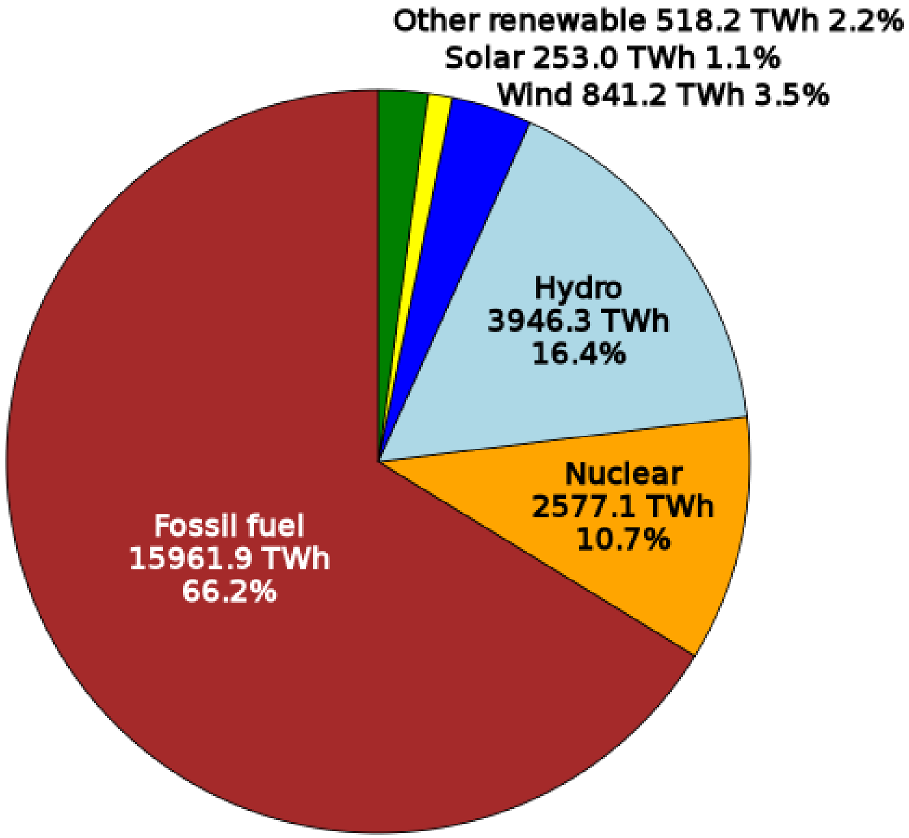






https://en.wikipedia.org/wiki/Climate_change

Alternatives to fossil fuels



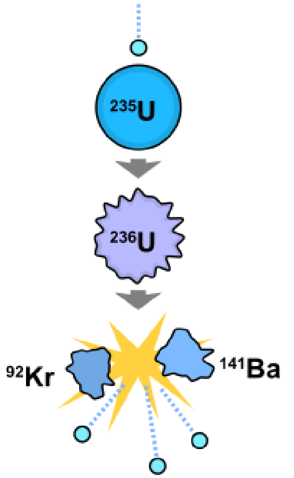
World Electricity Generation by Source (2015)

Fossil fuels used for 2/3rd of electricity generation

Renewable (hydro, geothermal, solar, wind)

- abundant & renewable
- cleaner than coal

- low power density
- reliability & energy storage



Nuclear fission

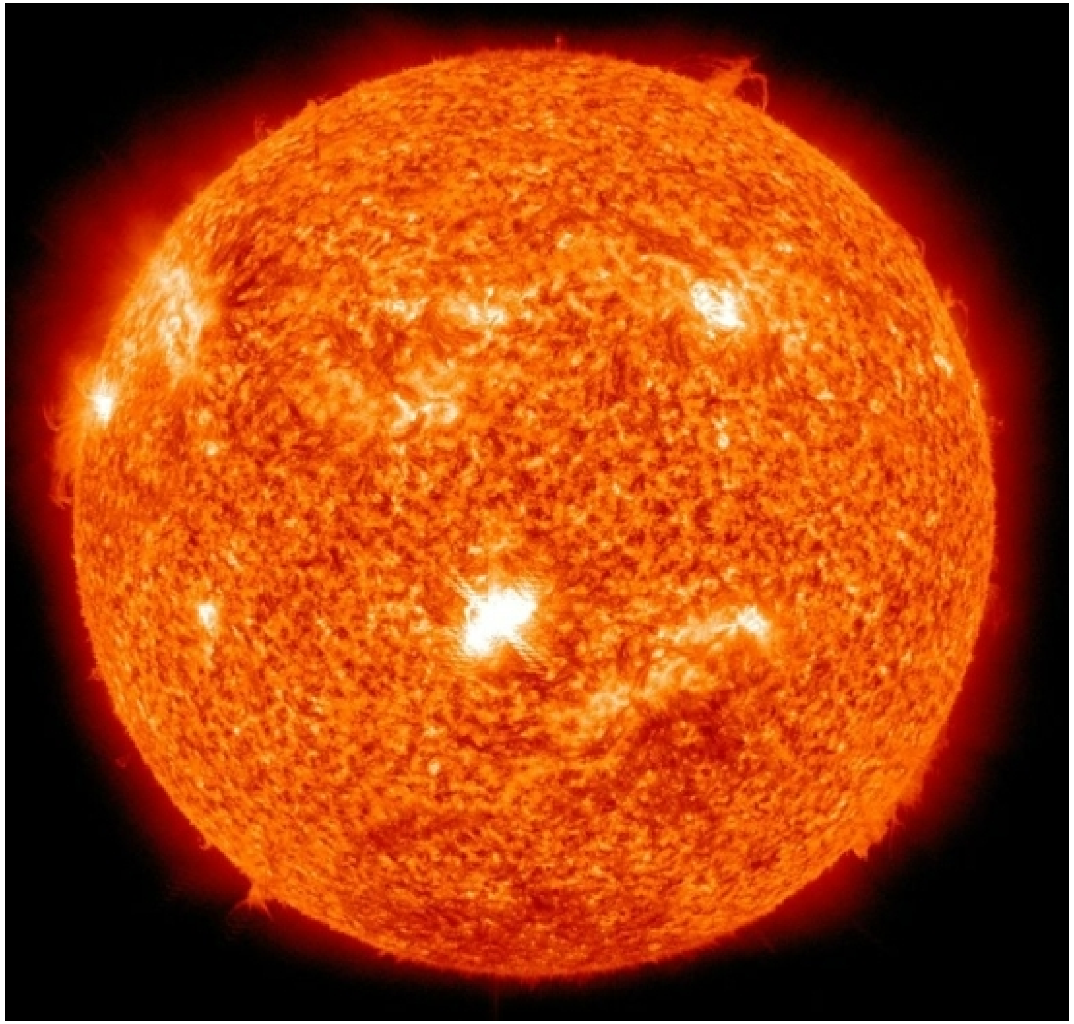
- low carbon emissions
- high power density

- radioactive waste storage
- expensive

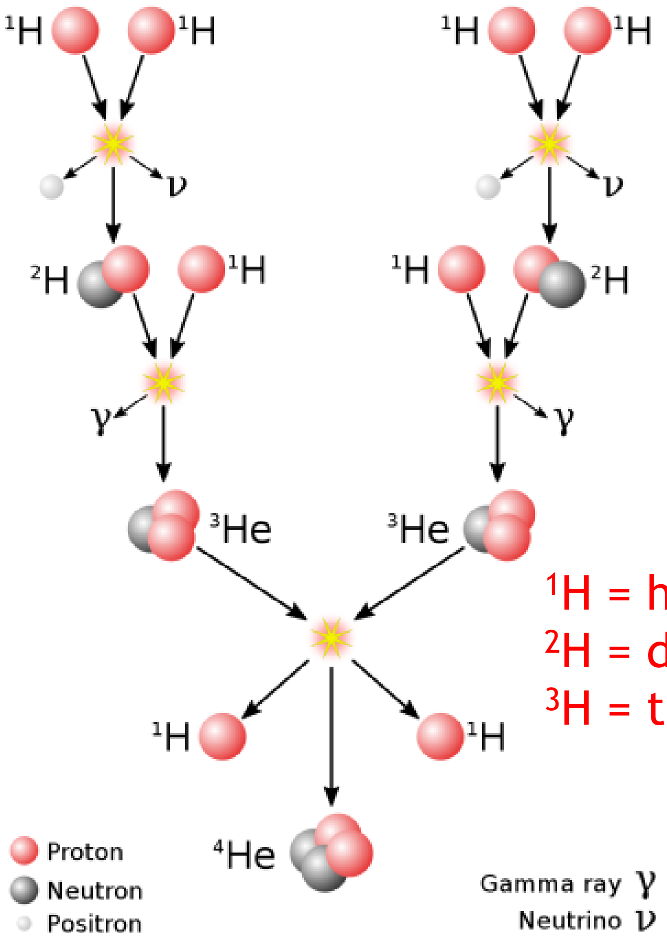
What about fusion energy?

What is fusion energy?

Fusion is the source of power for the Sun



atoms “fuse” together, releasing energy



^1H = hydrogen (H) (protium)
^2H = deuterium (D)
^3H = tritium (T)

https://en.wikipedia.org/wiki/Nuclear_fusion

Why fusion energy?

- Carbon free
- Avoids most radioactive waste problems from nuclear fission
- No risk of melt-down
- Not intermittent like wind and solar
- Abundant, nearly inexhaustible fuel supply of ^{2}H and Li
- Really difficult to achieve (ongoing research topic for 60+ years)
- Not ready yet—too long term to help fight against climate change?

To generate ~500,000 kWh of energy…

100 tons of coal

OR

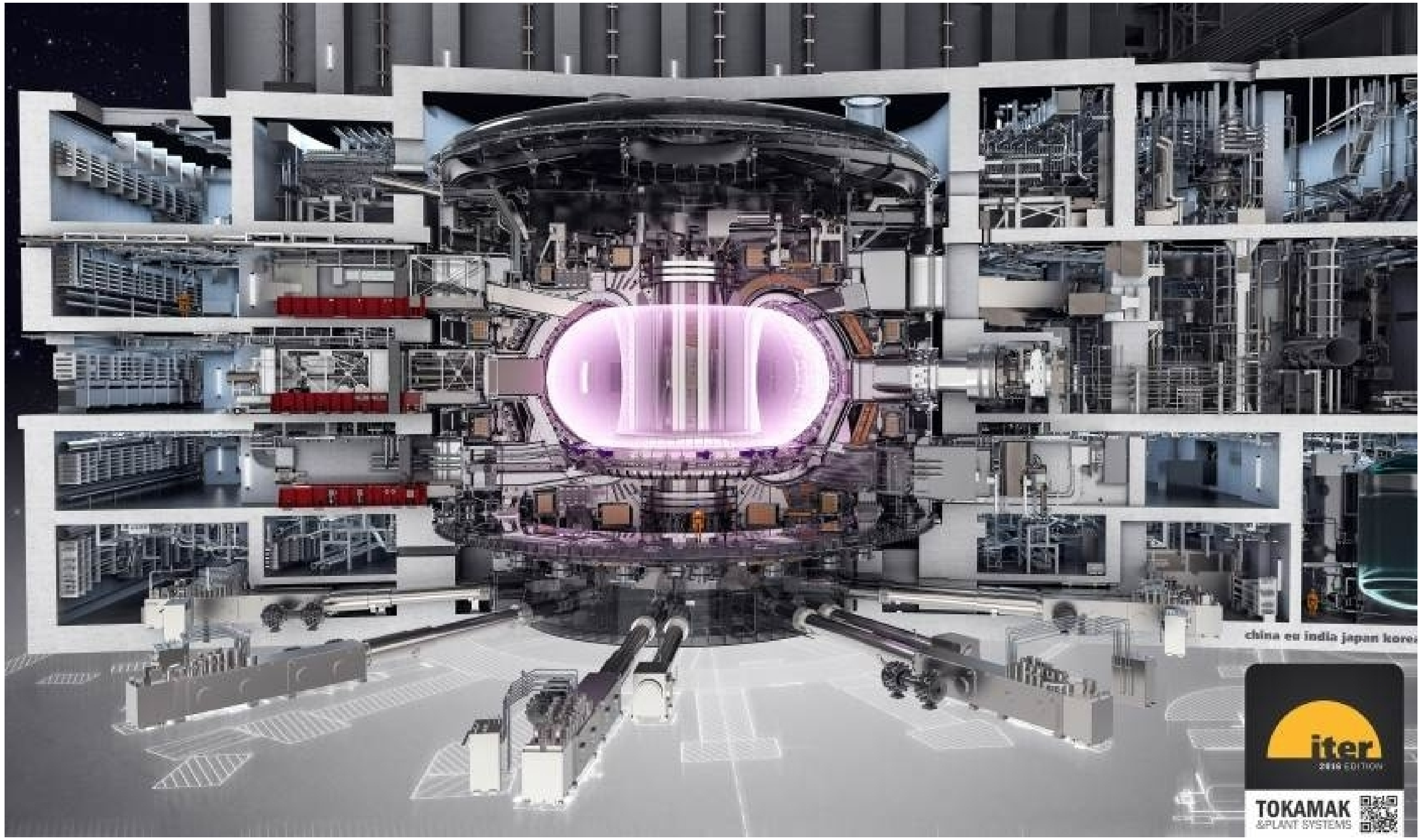
Lithium in 2 laptop batteries

+

50 gallons of water

How will we generate fusion energy on Earth?

Confine a "miniature Sun" in a reactor



Test reactor being built: International Thermonuclear Experimental Reactor

Fusion in a reactor

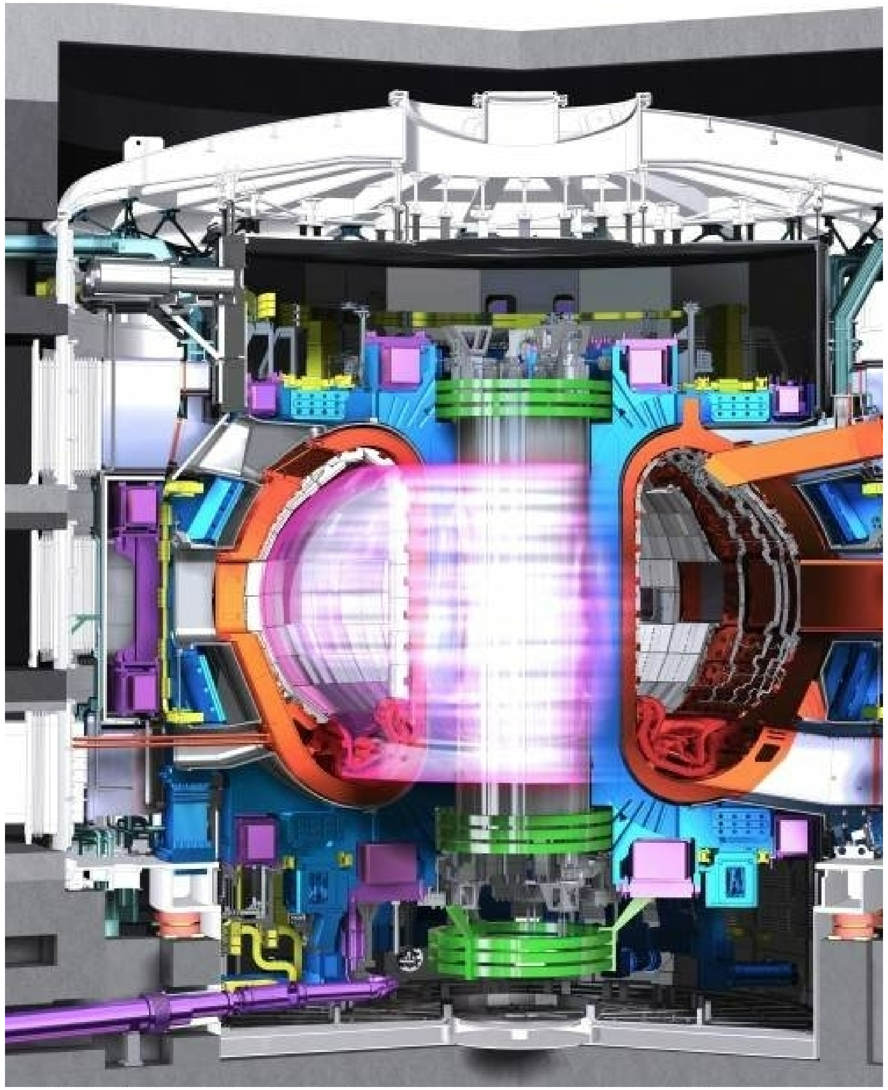
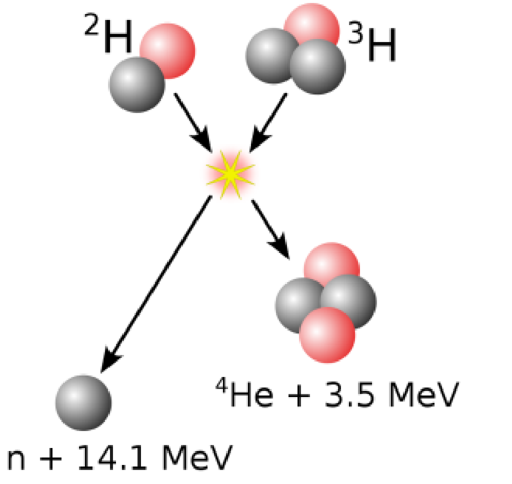


Image: iter.org

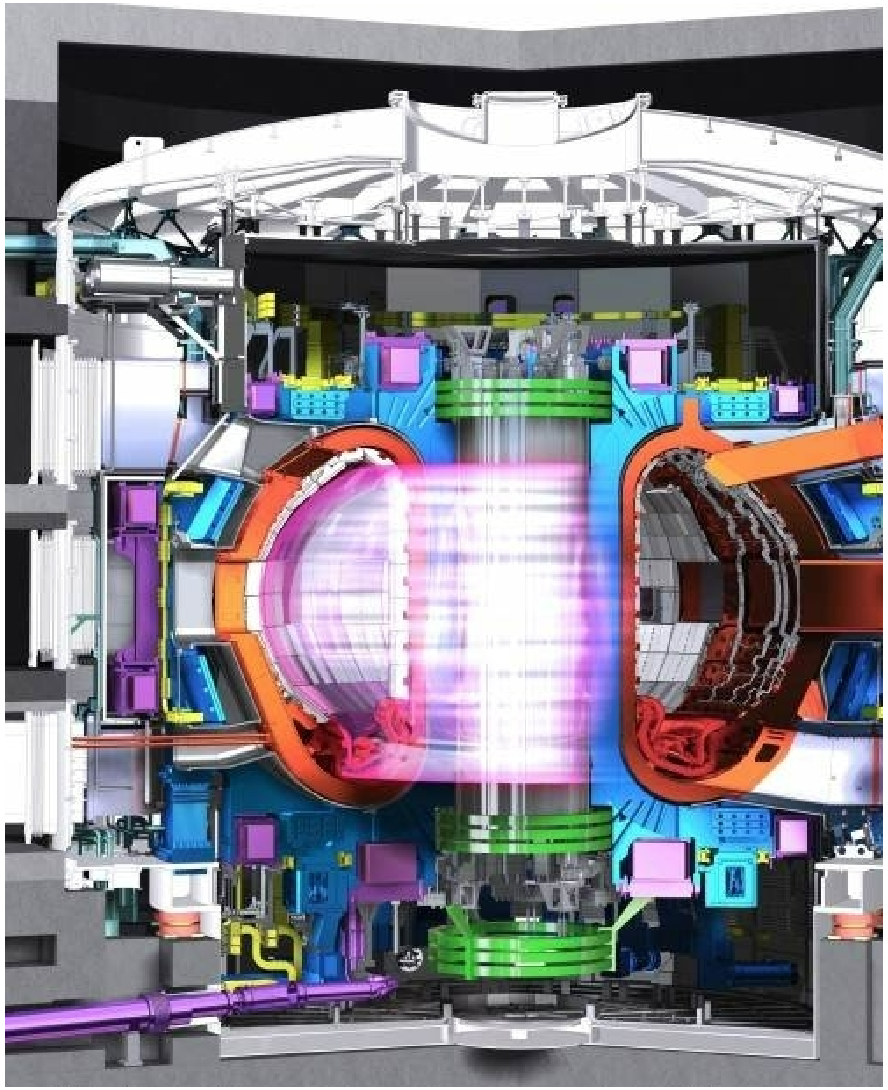


Fusion reaction:

D + T → He + neutron (14.1 MeV)

requires confinement of extremely hot (>100,000,000 ºC) plasma

Fusion in a reactor



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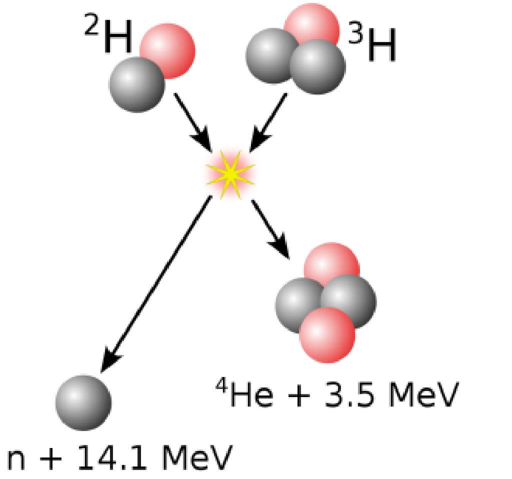

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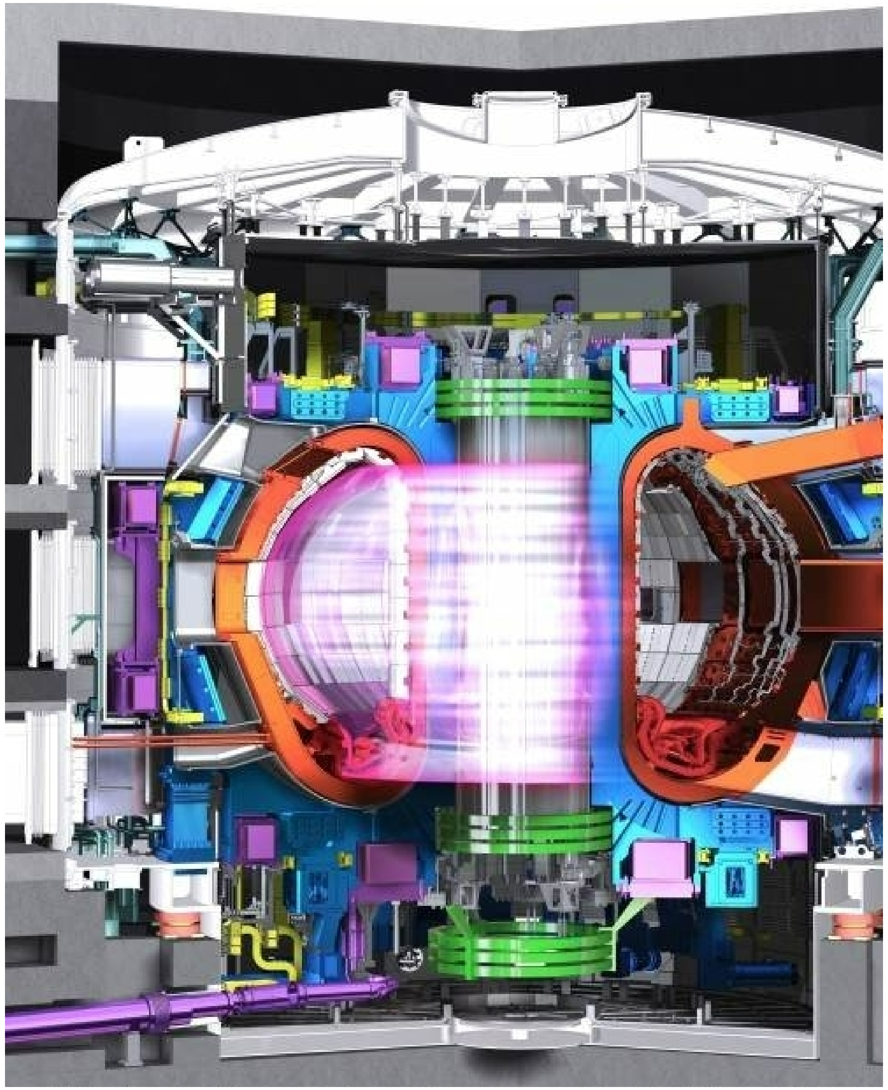
ionized gas: mixture of ions, electrons, & neutrals

Fusion in a reactor



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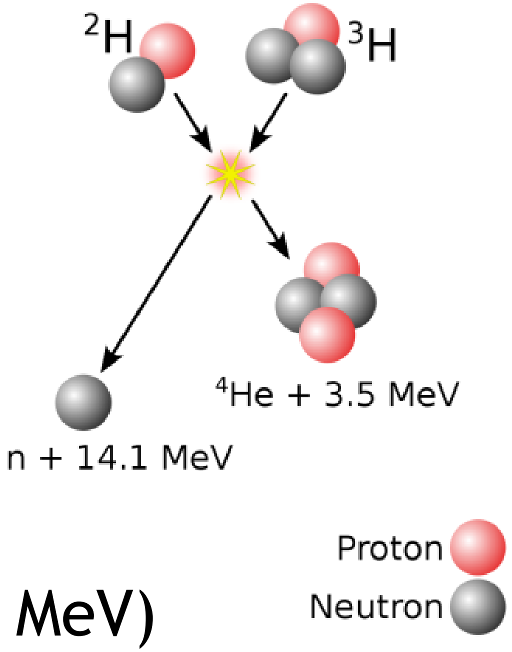


Fusion reaction:

D + T → He + neutron (14.1 MeV)

requires confinement of extremely hot ([illegible]00,000,000 ºC) plasma

Note: tritium (^{3}H) is radioactive, with a short half-life (~13 years)

- Radiological health concern
- Hard to store T, we will need to "breed" T in the reactor

Fusion in a reactor

Fusion triple product:

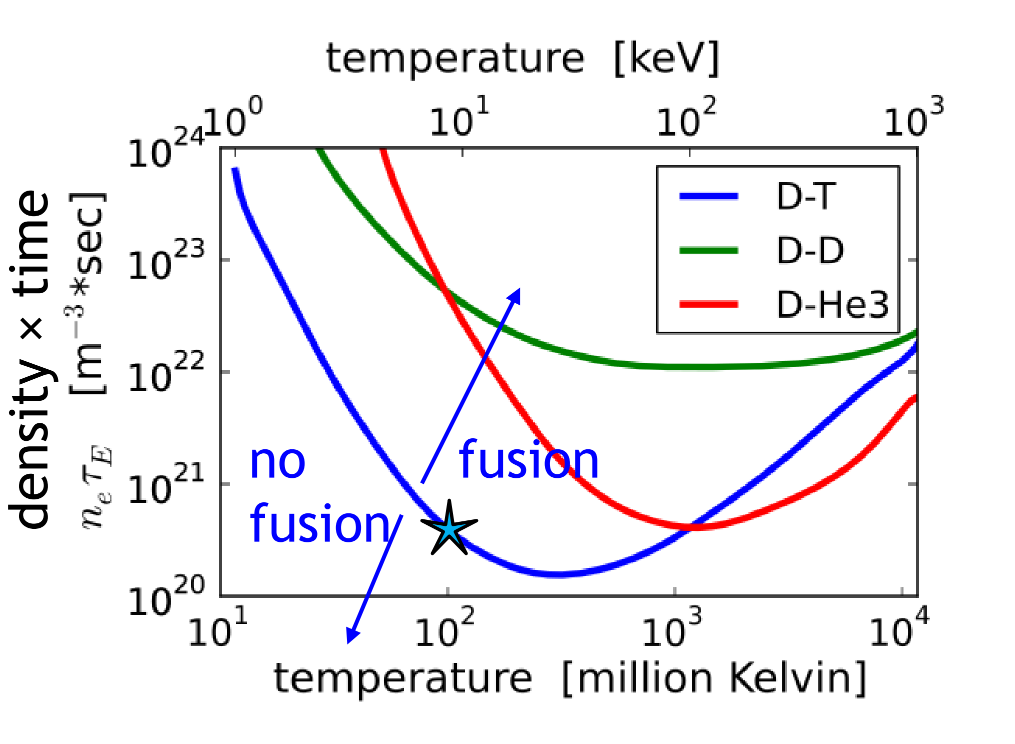
For fusion to be self-sustaining, need to maximize:

- density (n) × confinement time (τ) × temperature (T)
- varies with fusion species
- T: overcoming repulsion between protons
- n, τ: sufficient fusion events to sustain temperature

For D-T fusion at 100 million °C, $n\tau > 3 \times 10^{20}$ m^{-3} s

- optimal $n \approx 10^{19}$ m^{-3} (10^{-6} atmospheric pressure)
- required $\tau > 30$ seconds

Lawson criteria:



D-T has lowest $n\tau T$ requirement

Quick overview of a tokamak

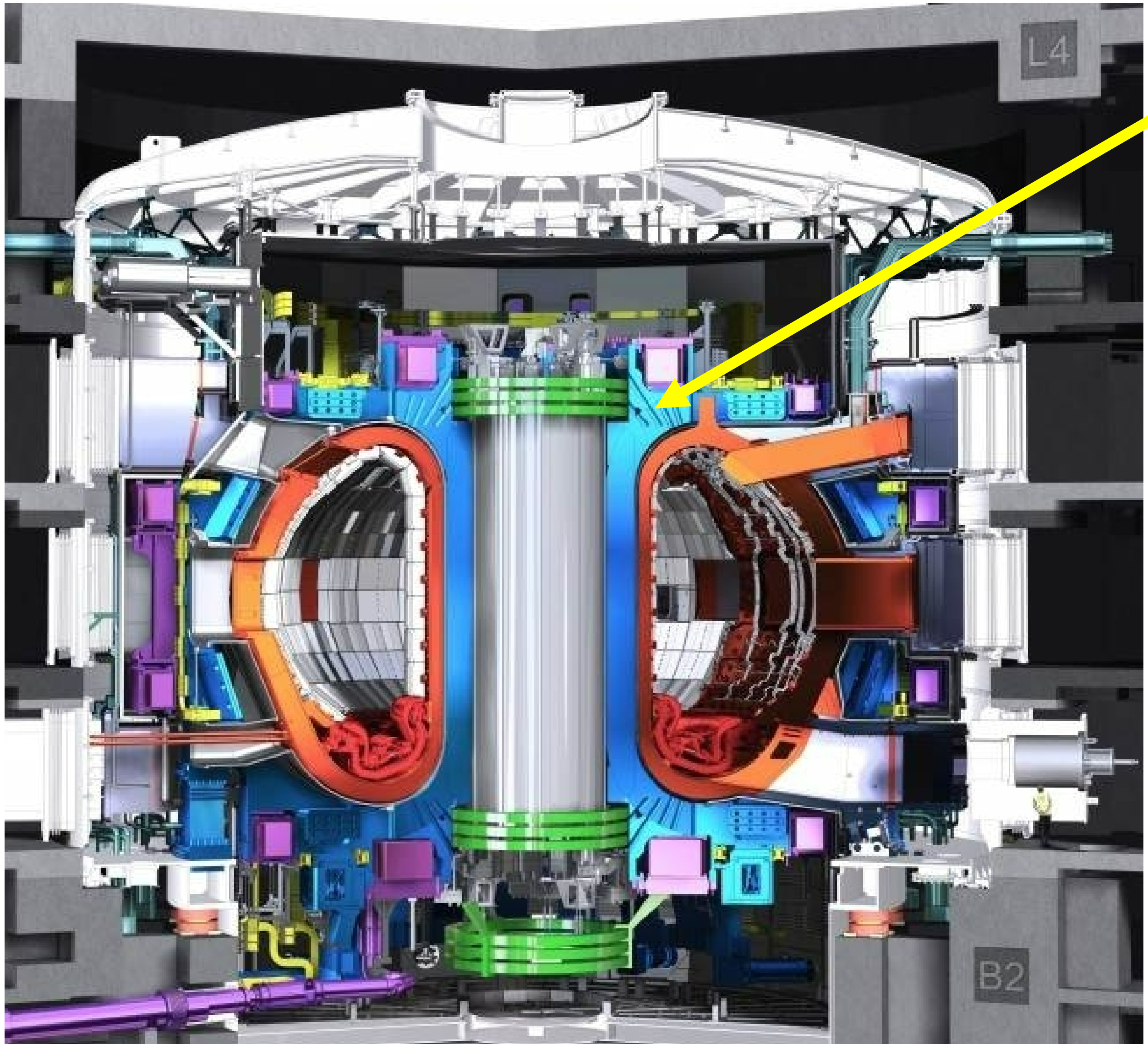


Image: iter.org

Plasma confinement

Plasma is confined by magnetic fields shaped by superconducting magnets

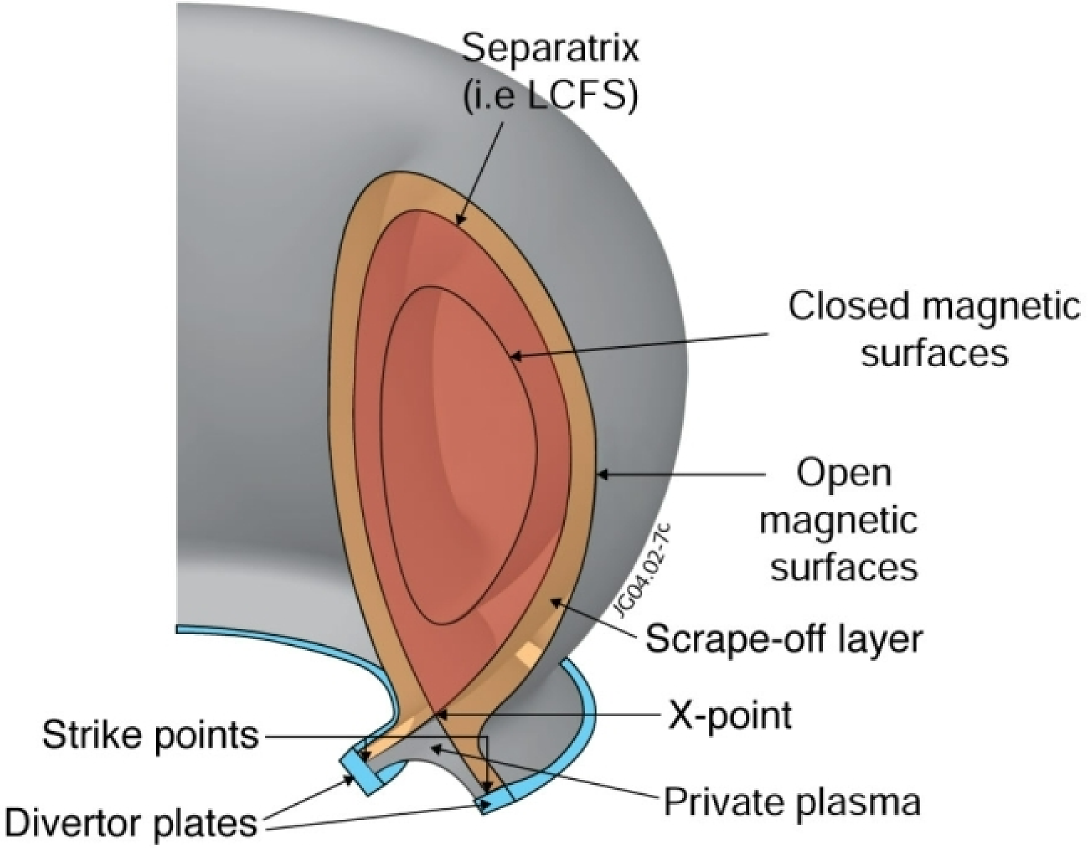
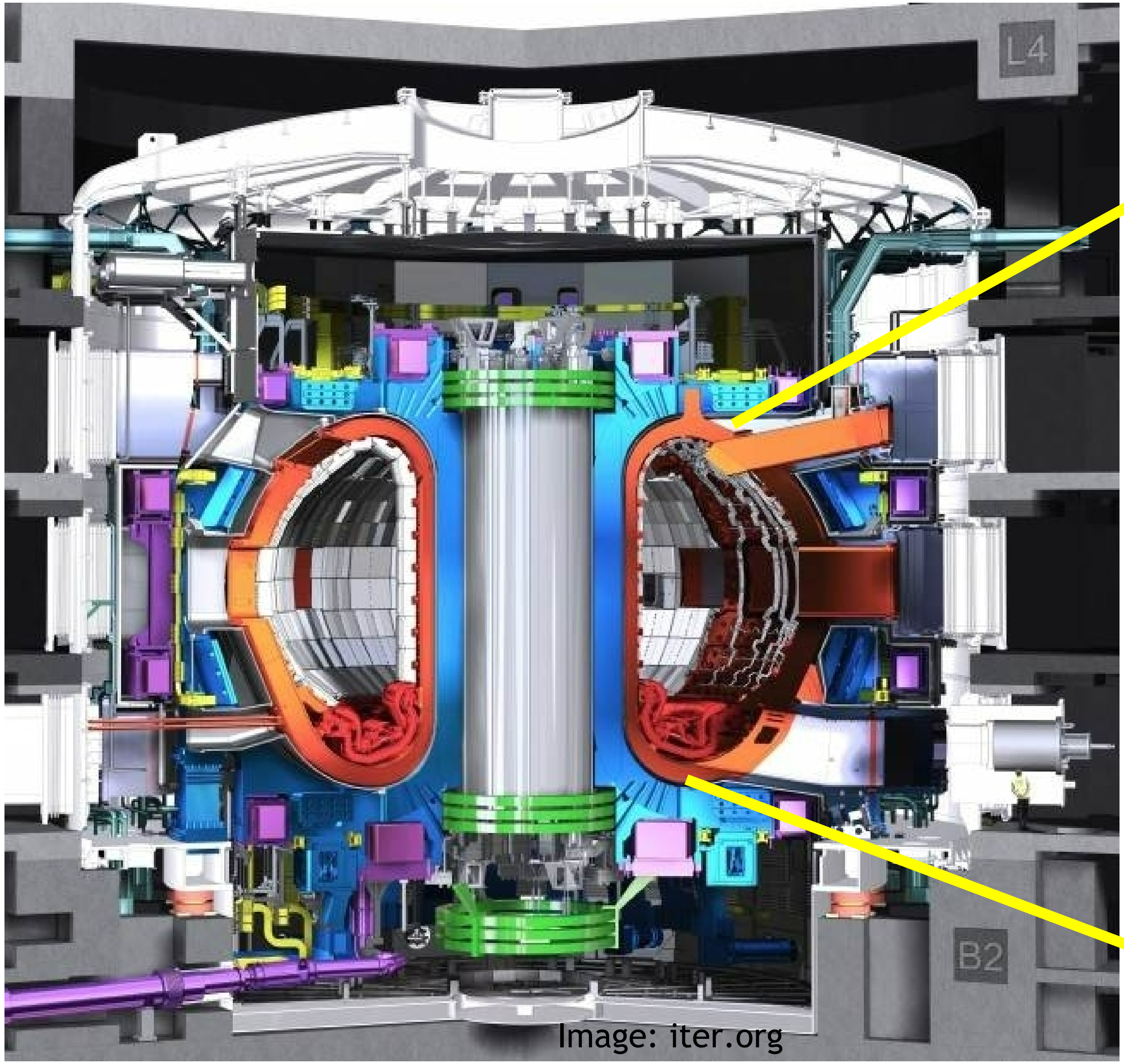


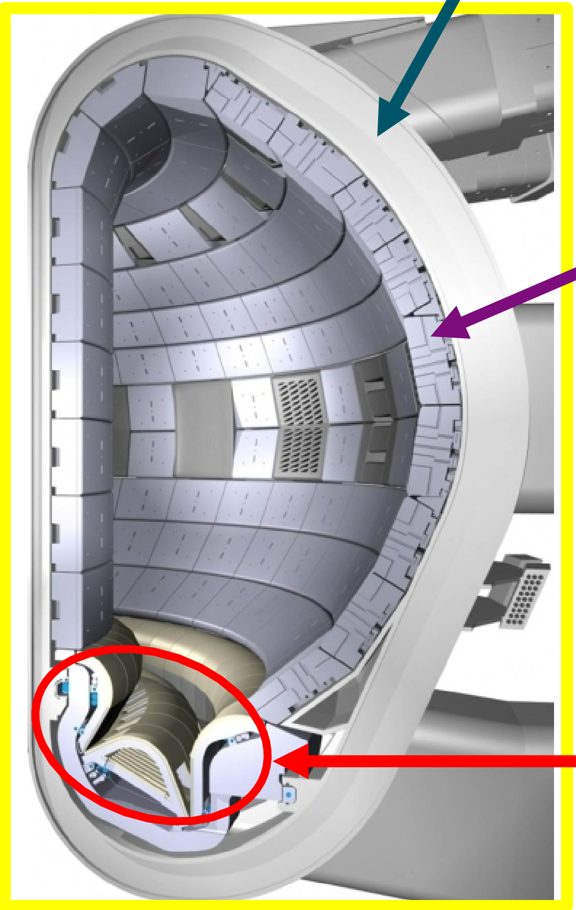
Image: euro-fusion.org

Quick overview of a tokamak



Stainless steel structure

Vacuum vessel



Blanket:
- protects stainless steel structure
- responsible for breeding tritium

Divertor:
- “trash can”
- particles & heat dumped here

What materials can be used in the divertor?

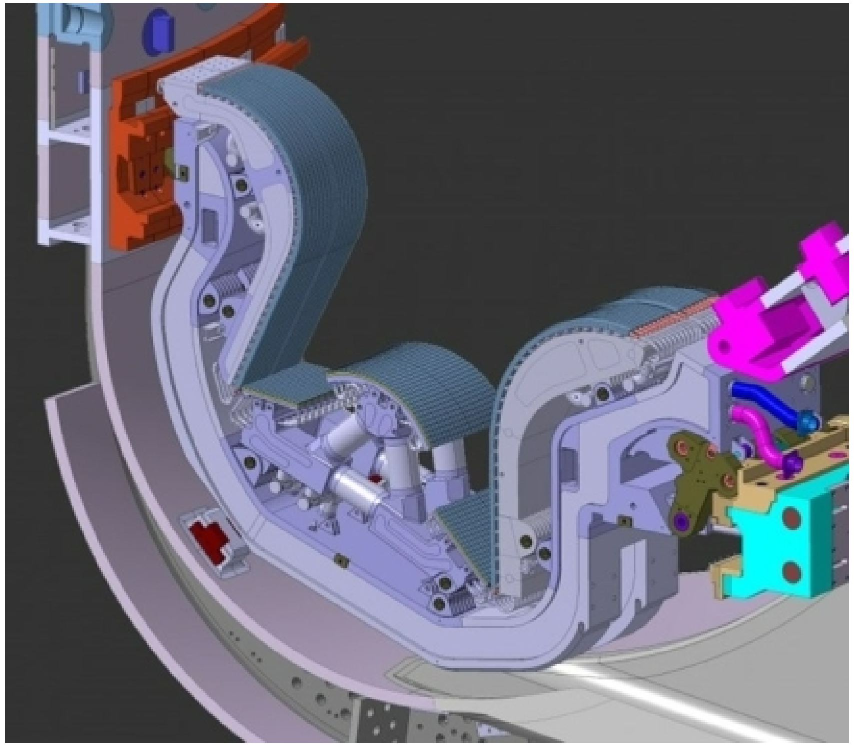


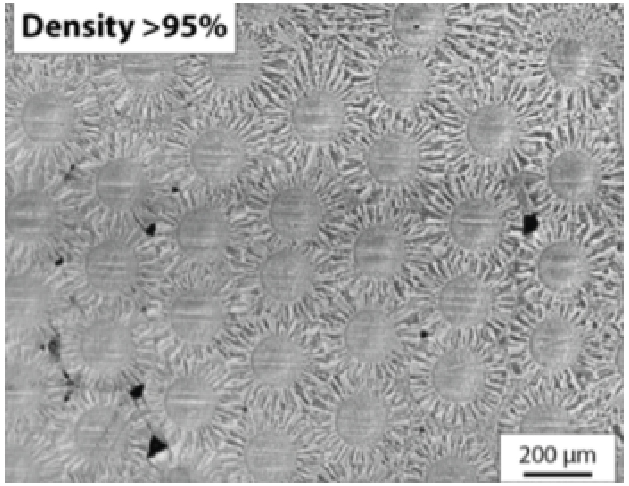
Image: iter.org

tungsten is a leading candidate material

- highest melting point
- low sputter yield
- high thermal conductivity

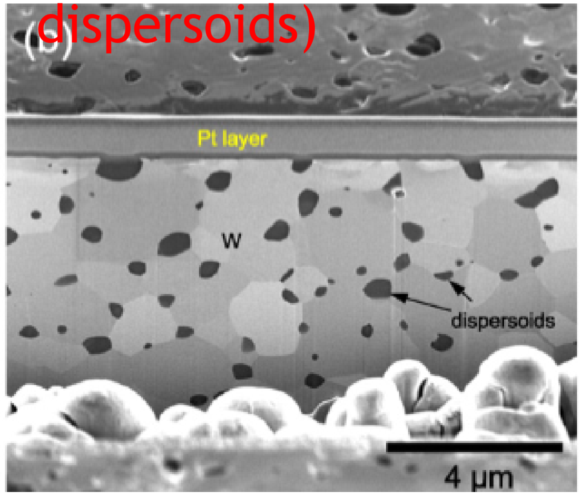
active area of research, as polycrystalline W is likely insufficient for a commercial reactor

W-fiber reinforced W



J. Coenen et al. IAEA - FEC2014

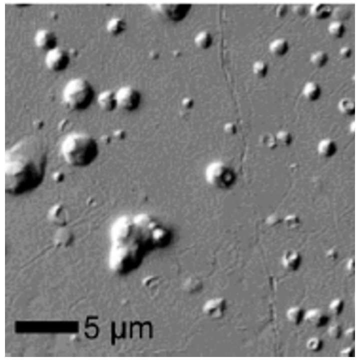
UFG-W (Ti dispersoids)



Kolasinski et al., IJRMHM, (2016).

(some) Key materials challenges for a fusion reactor

D-blistering on W



Kolasinski et al.,
J App. Phys. (2015).

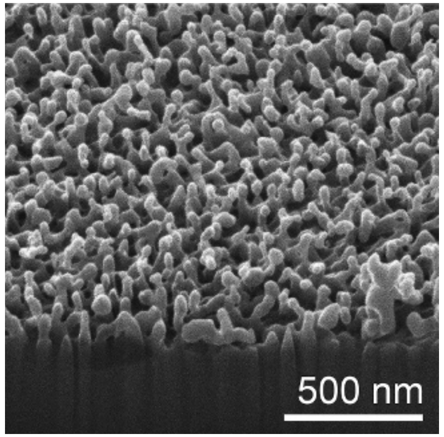
deuterium & tritium

- H embrittlement & blistering
- T retention (radiological hazard)
- T breeding & separation

helium

- bubble formation
- fuzz growth

tungsten fuzz



Wong et al.,
Nucl. Mater. Energy (2020).

Fusion reaction:

$$D + T \rightarrow He + n^0 \ (14.1 \text{ MeV})$$

confinement of hot plasma with impurities (e.g. N)

neutrons

- displacement damage
- transmutation (e.g. W → Re or Li → T)

impurities

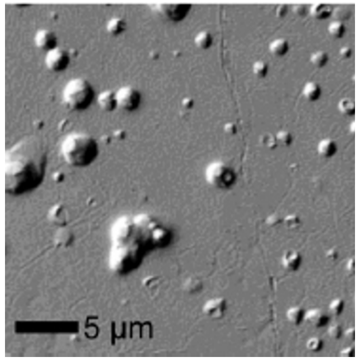
- chemically enhanced sputtering
- formation of active species e.g. NH_3

heat

- recrystallization (weakens materials)
- even melting of tungsten predicted

(some) Key materials challenges for a fusion reactor

D-blistering on W



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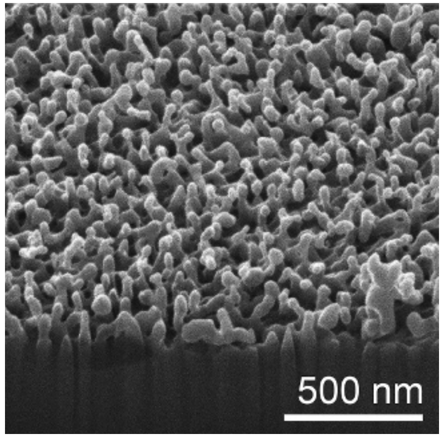

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My work: how do hydrogen & helium interact with tungsten surfaces?

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- What is fusion and how does it work?
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Low energy ion beam analysis of material surfaces

- **Hydrogen adsorption on tungsten(111)**
- Structural studies of tungsten(111) to understand defect nucleation & growth
- Ongoing/future work
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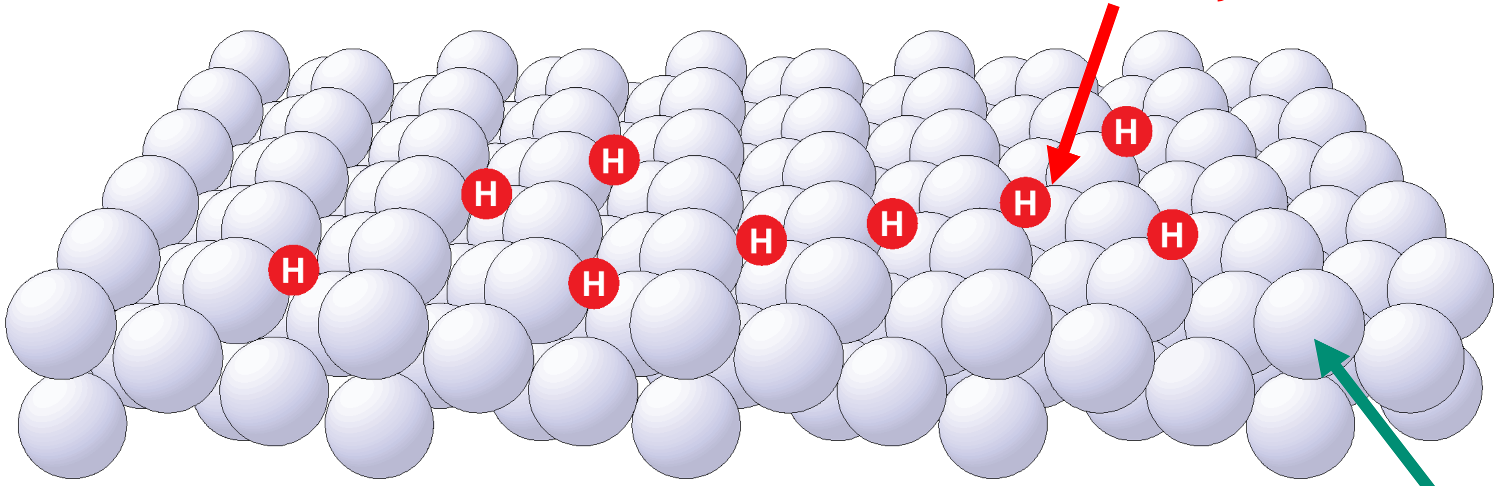
Summary

Hydrogen on tungsten surfaces

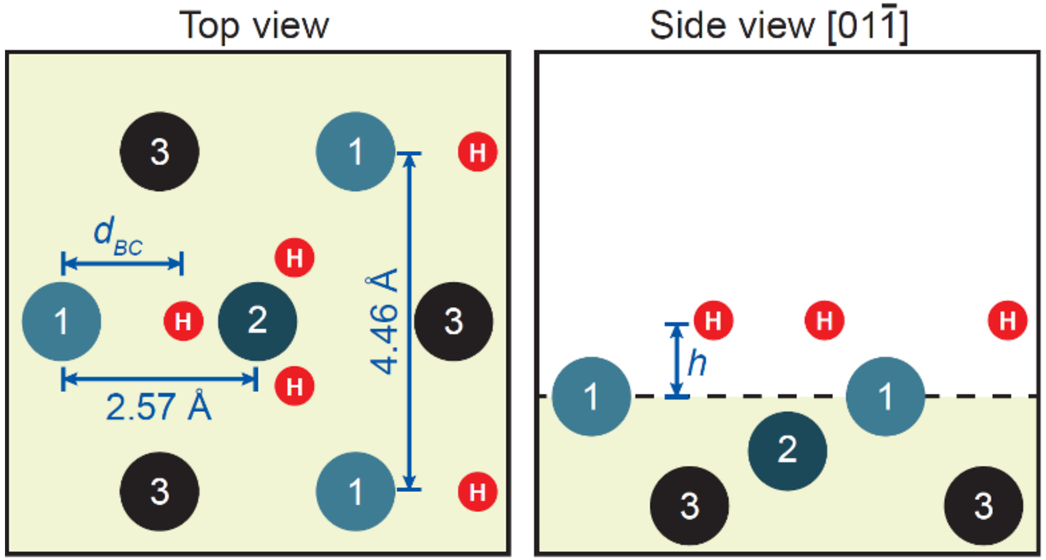
Hydrogen will get adsorbed on tungsten surfaces, but where exactly does the H bind?



To validate model predictions, we need to determine hydrogen location with ~0.01 nanometer precision (30× smaller than the spacing between W atoms!)

DFT can provide insight into hydrogen-tungsten interactions

Bond centered (BC) site on W(111) predicted using density functional theory (DFT) by our collaborators: Zack Bergstrom and Brian Wirth at University of Tennessee



$1.5\ Å \leq d_{BC} \leq 1.7\ Å$ $0.95\ Å \leq h \leq 1.10\ Å$

We would like to experimentally validate their results, since:

DFT provides inputs for larger scale models

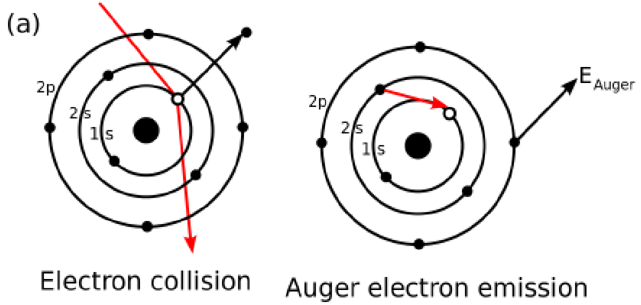
- interatomic potentials (H + W)
- dissociation & recombination of H

Z. Bergstrom et al., J. Phys. Condens. Matter, (2019).

Challenges for detecting surface H

LEED

AES

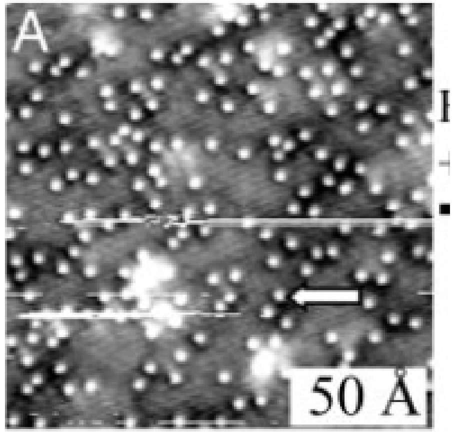


wikipedia.org

Direct detection of surface H is challenging:

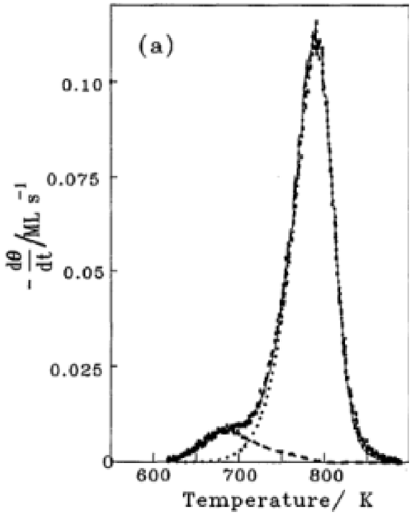
- Direct detection impossible for many techniques (XPS, AES)
- Challenging to disentangle H signal from substrate (LEED, STM, HAS)
- Ambiguous surface/location information (TPD)

STM



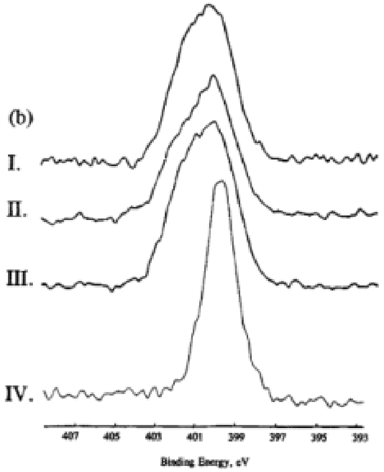
Sykes et al., PNAS (2005).

TPD



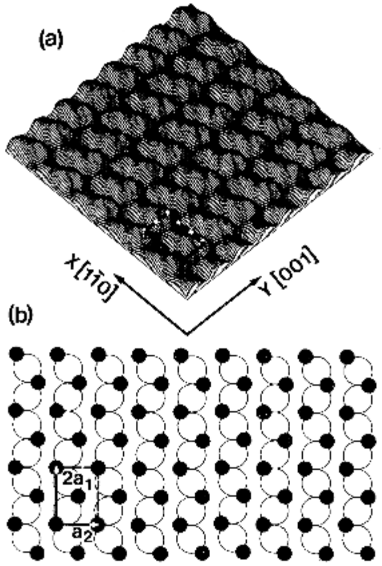
Flowers et al., J. Chem. Phys. (1993).

XPS



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

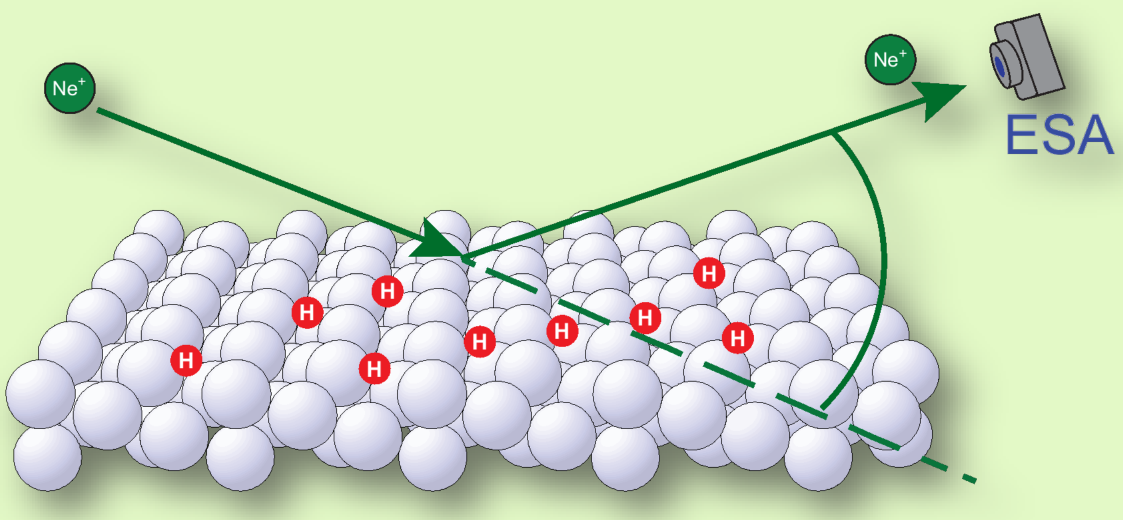
HAS



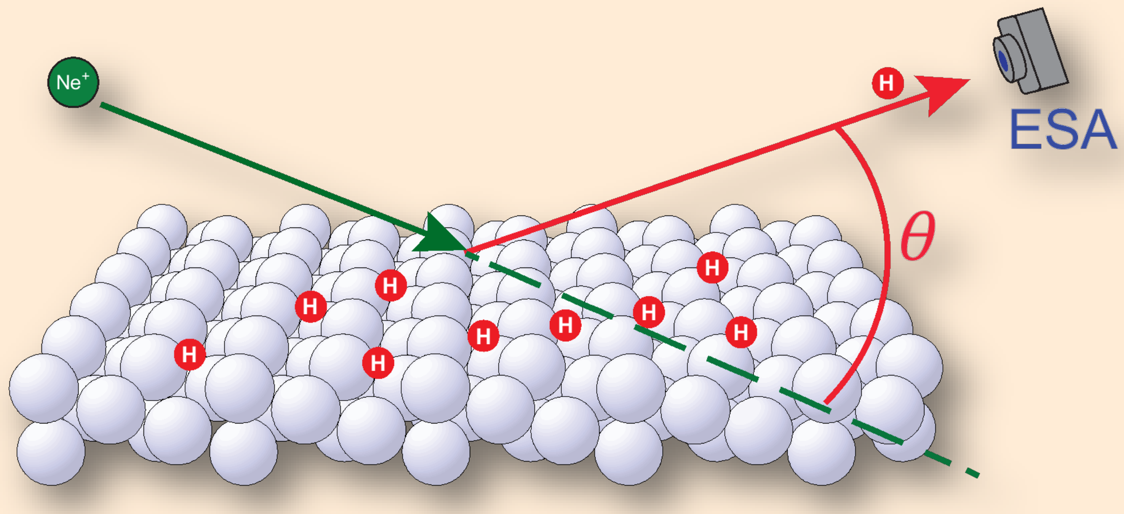
Rieder and Engel, PRL (1980)

LEIS and DRS for H detection

Low energy ion scattering (LEIS)

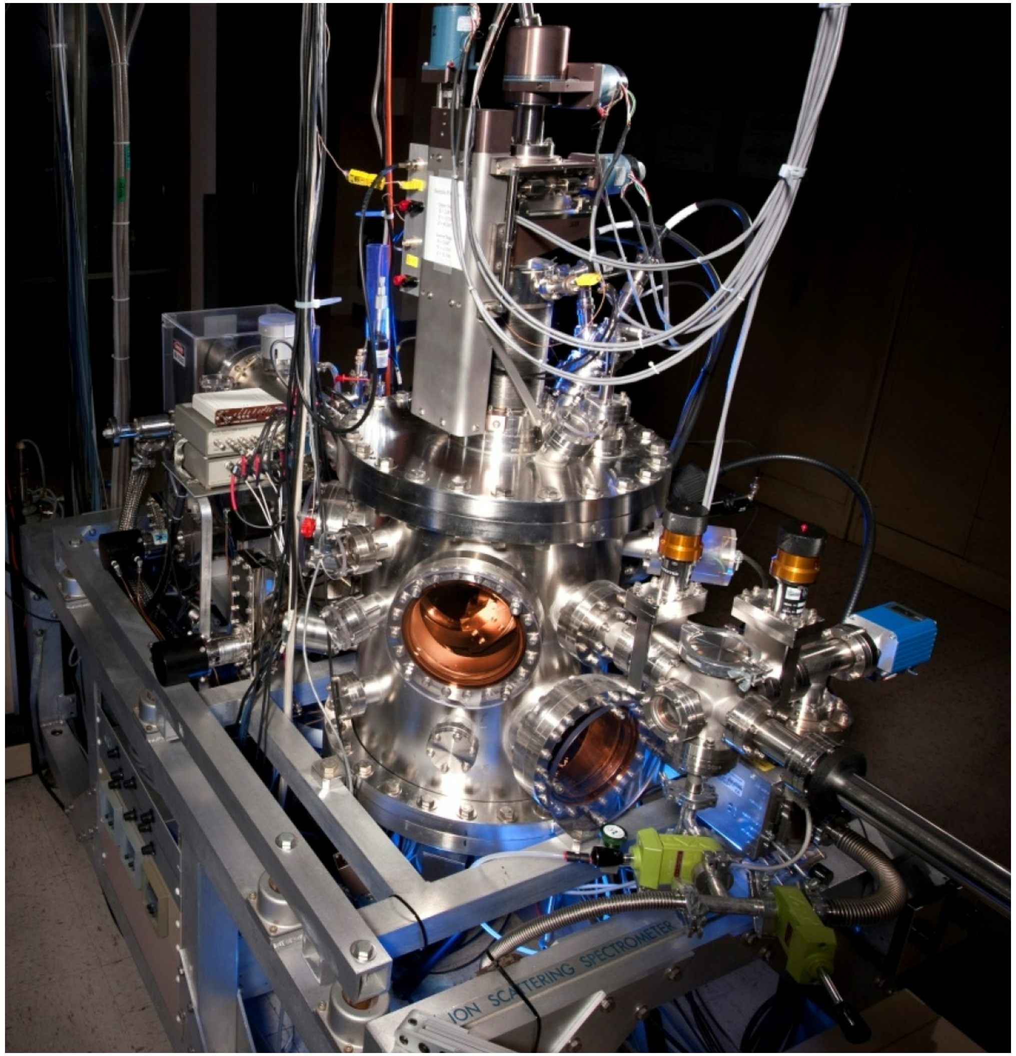


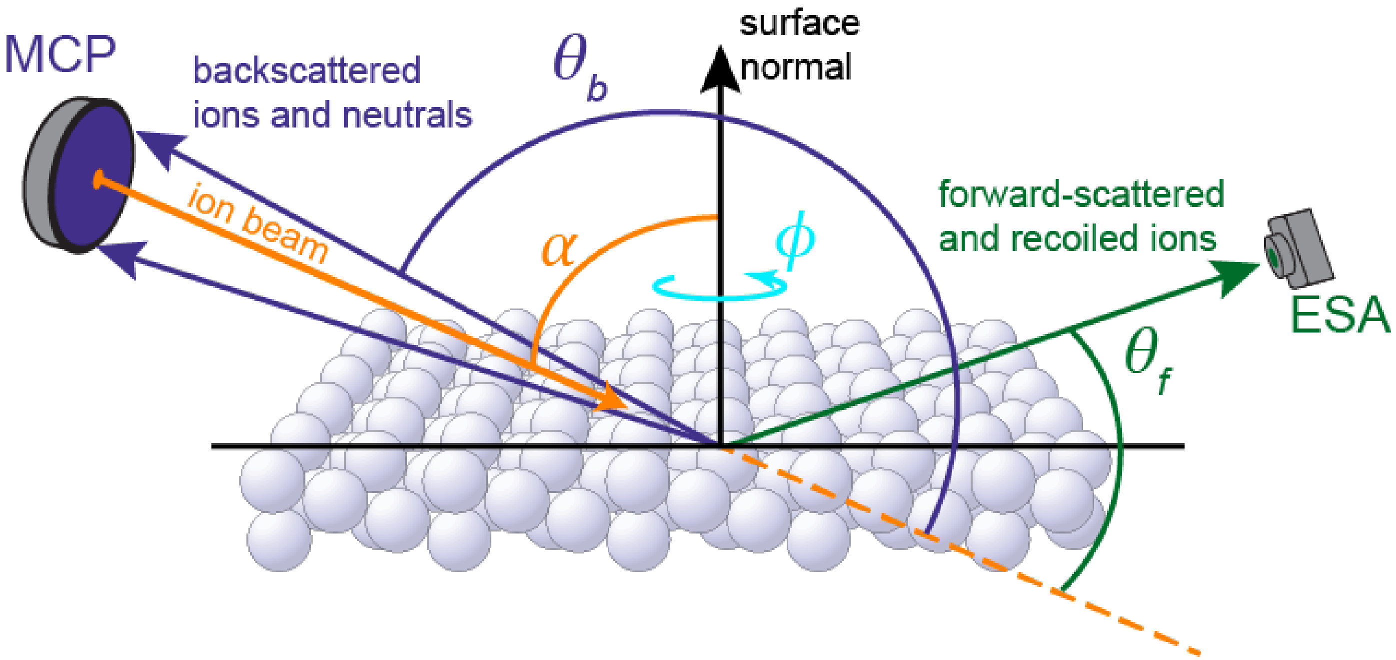
Direct recoil spectroscopy (DRS)



- both techniques are performed simultaneously
- energy of detected ion gives compositional information
  - elastic collision with conservation of momentum & energy (physics 1)

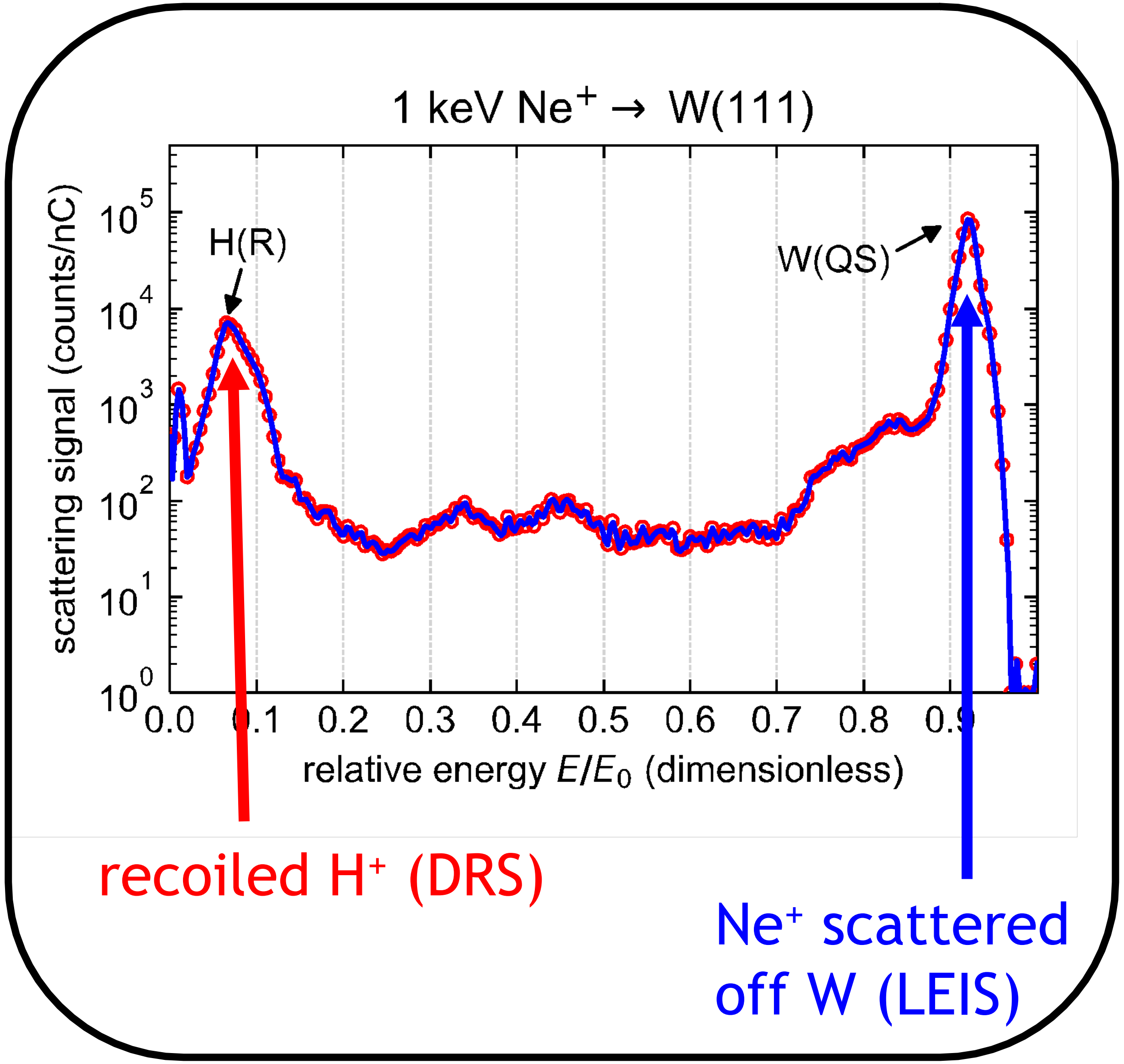
ARIES: Angle-Resolved Ion Energy Spectrometer





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

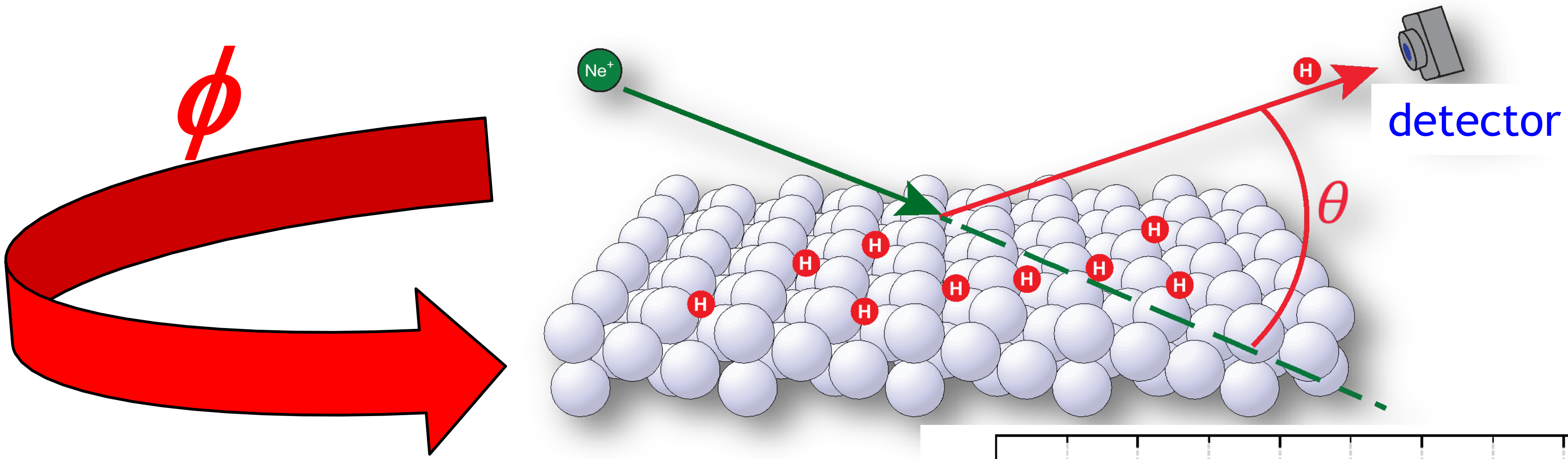
Ion energy spectrum for 1 keV $Ne^+ \rightarrow W(111)$



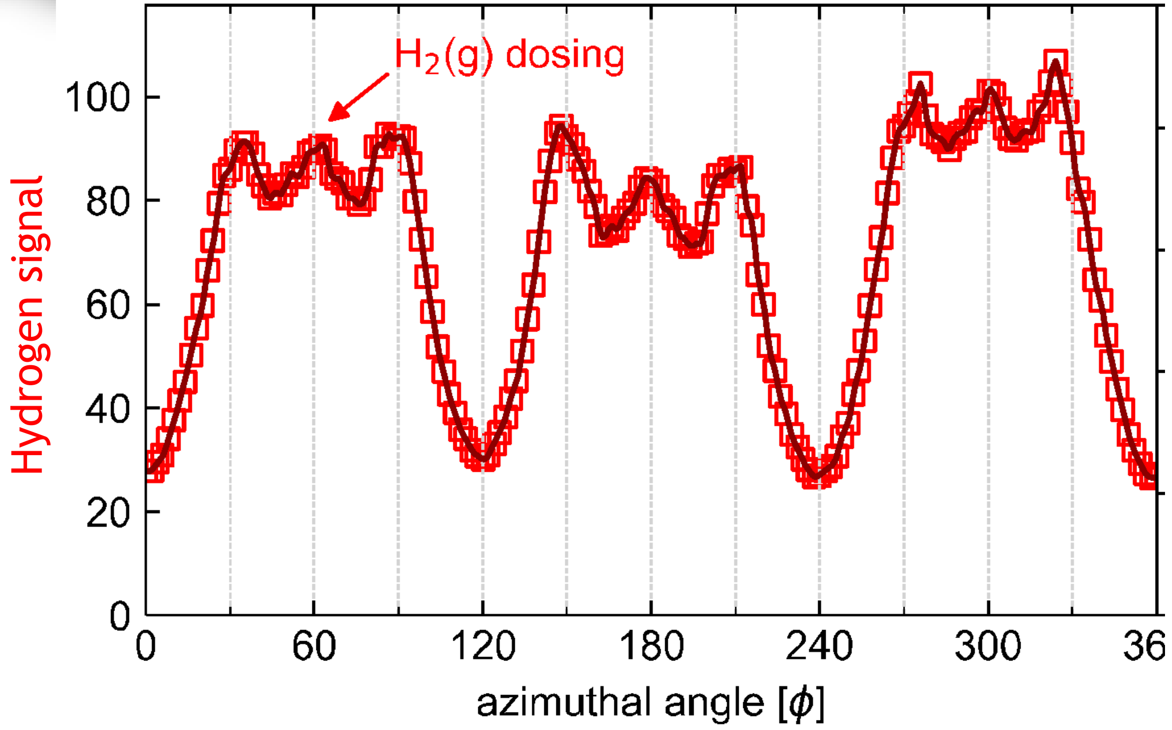
Key advantages of LEIS & DRS

1) direct detection of hydrogen on surface
2) structural information from W(QS) signal
3) surface specificity (monolayer sensitivity)

Hydrogen signal as we rotate the tungsten crystal



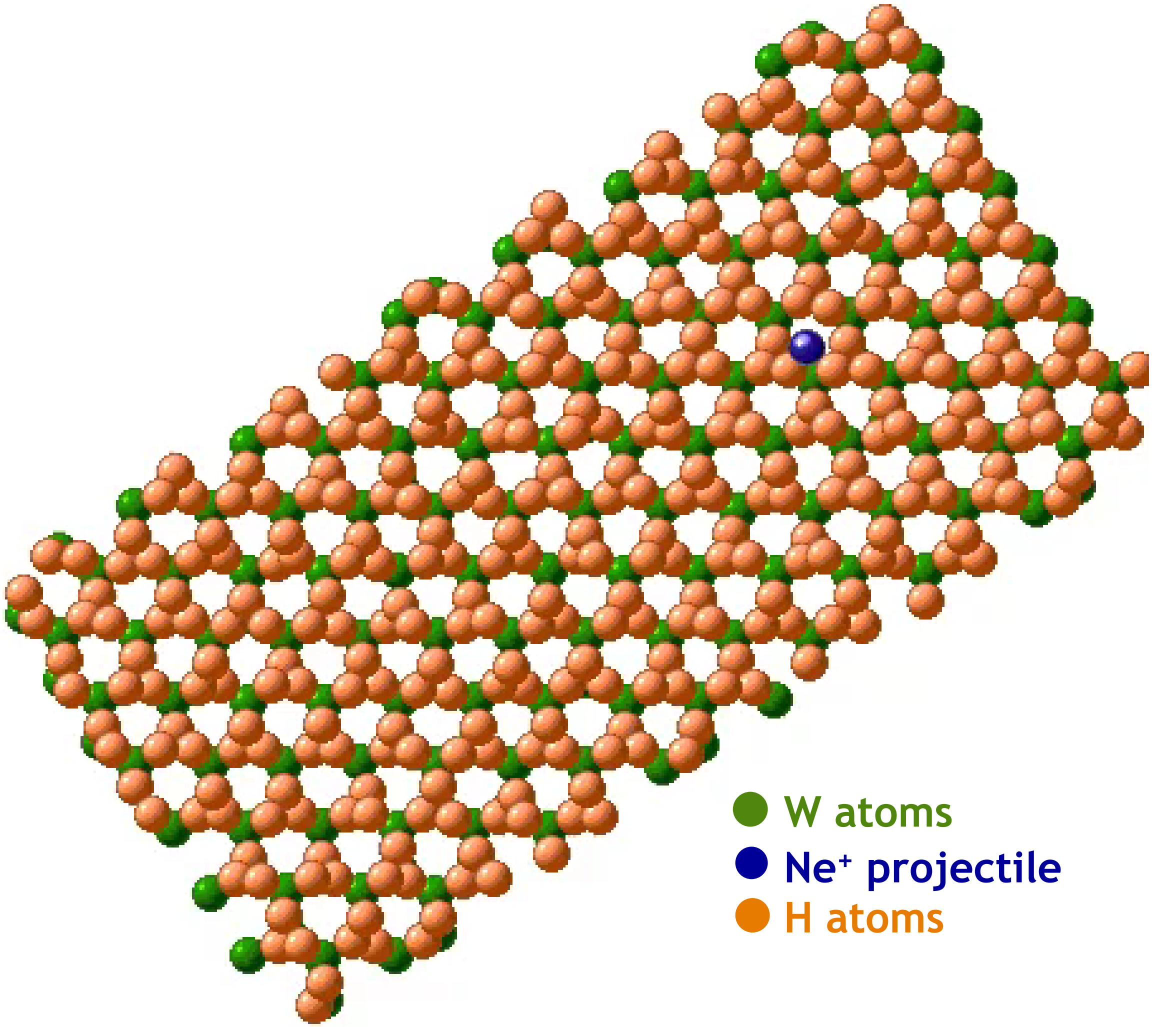
The hydrogen signal changes as we rotated the crystal around



Modeling experimental measurements

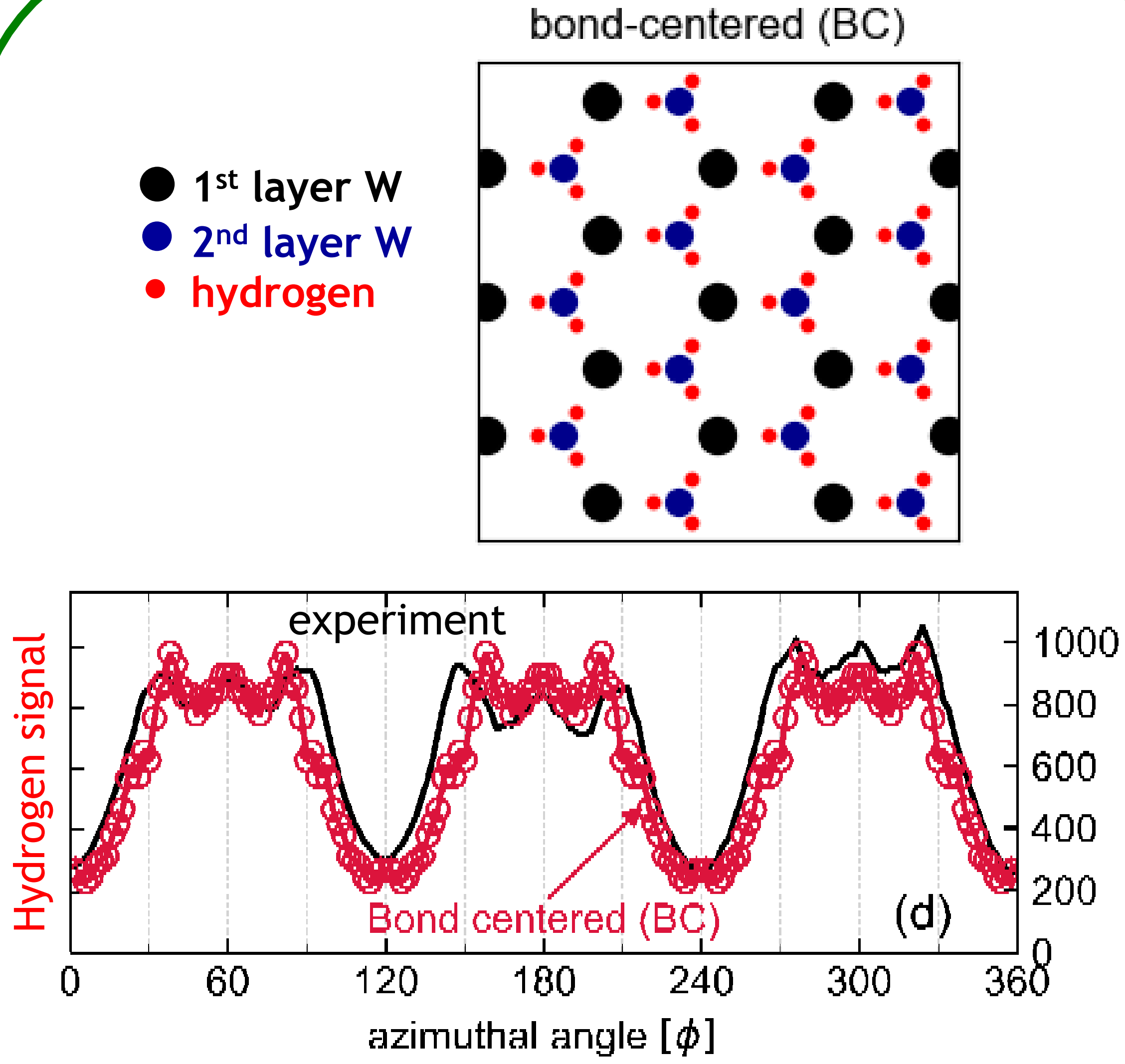
Experiments modeled with molecular dynamics simulations [1]

- Molecular dynamics—atoms are advanced in time according to F = ma
- 1 projectile at a time, target reset between projectiles
- Projectile interacts through ZBL potential (screened Coulomb) with target
- Count H that would reach the detector, as in the experiment

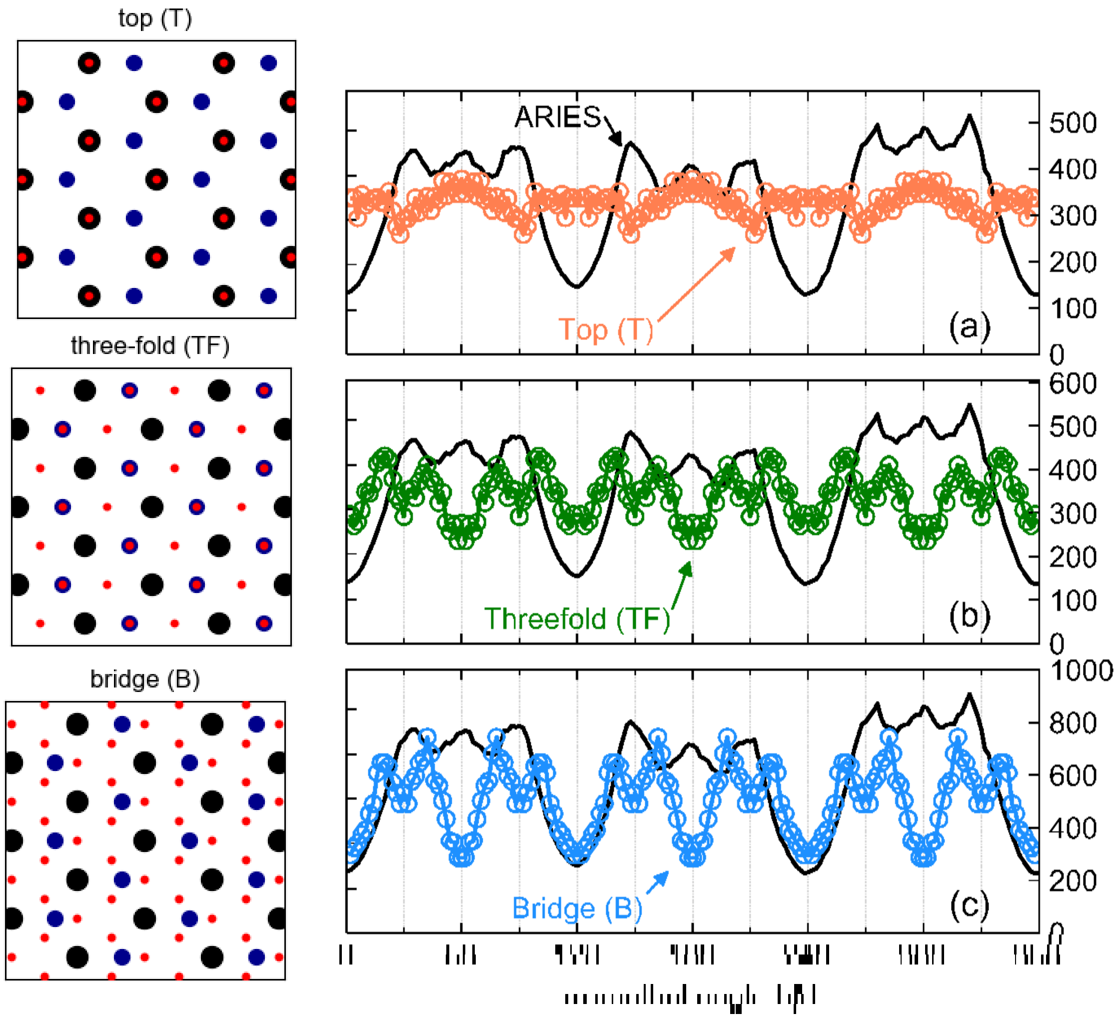


[1] Karolewski, Nucl. Instrum. Methods Phys. Res. B **230,** (2005).

Comparison of simulation to experiment



Other hydrogen locations

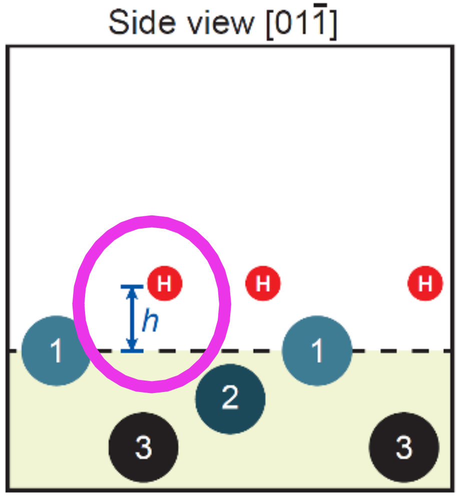


Constraining adsorbate height and posit

Model h = 1.0 ± 0.1 Å

DFT prediction:

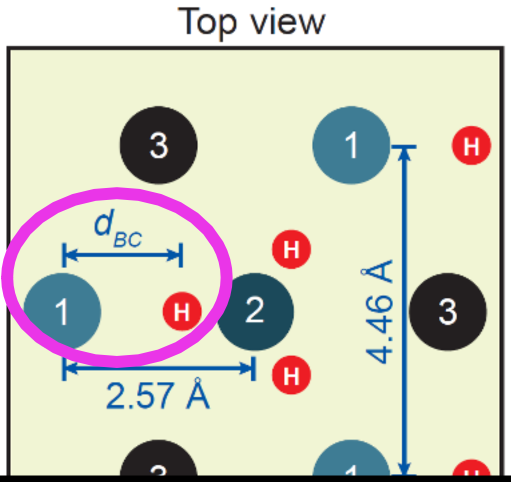
0.95 Å ≤ h ≤ 1.10 Å



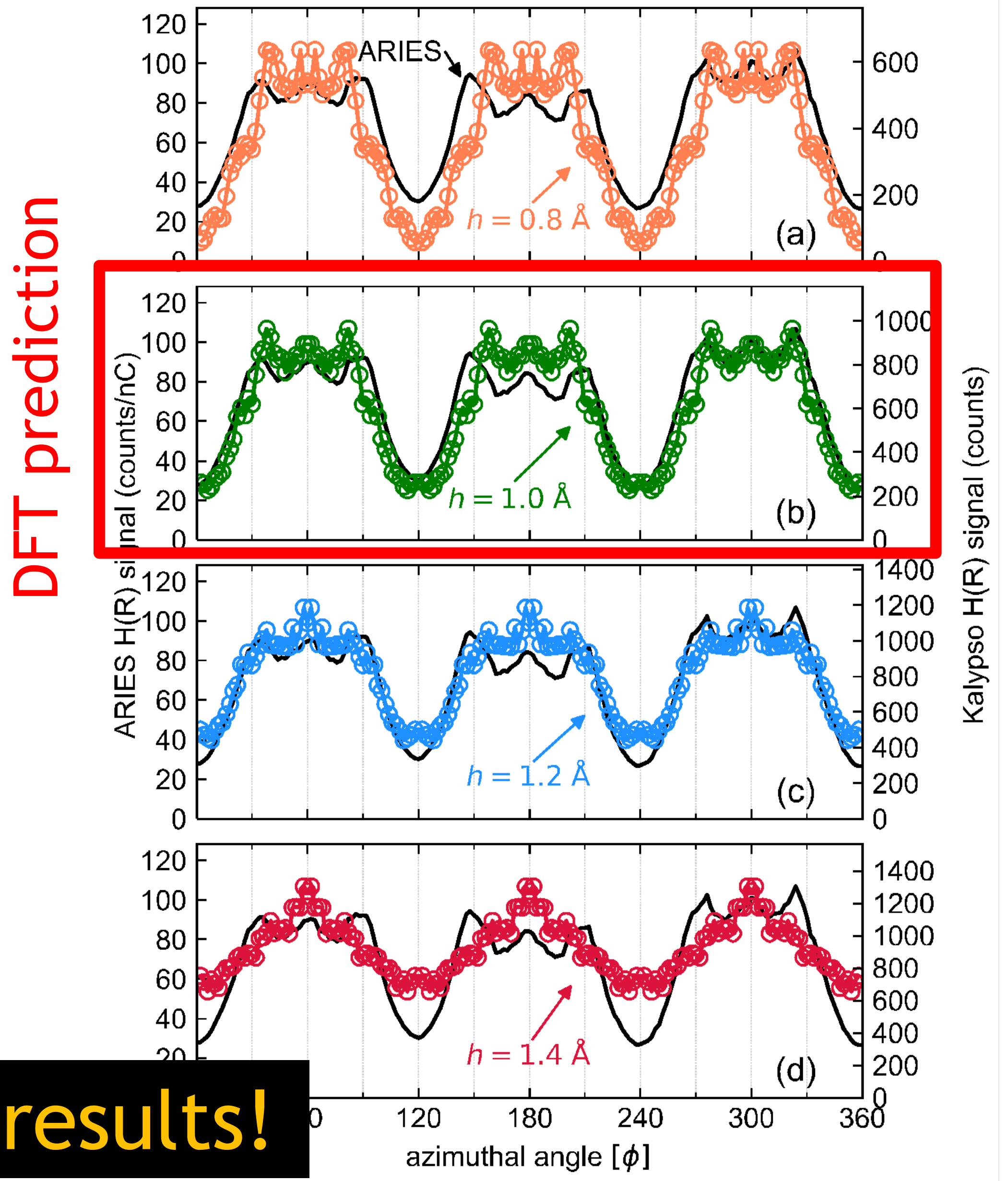
Model d_{BC} = 1.6 ± 0.1 Å

DFT prediction:

1.5 Å ≤ d_{BC} ≤ 1.7 Å



varying h



Strong validation of DFT results!

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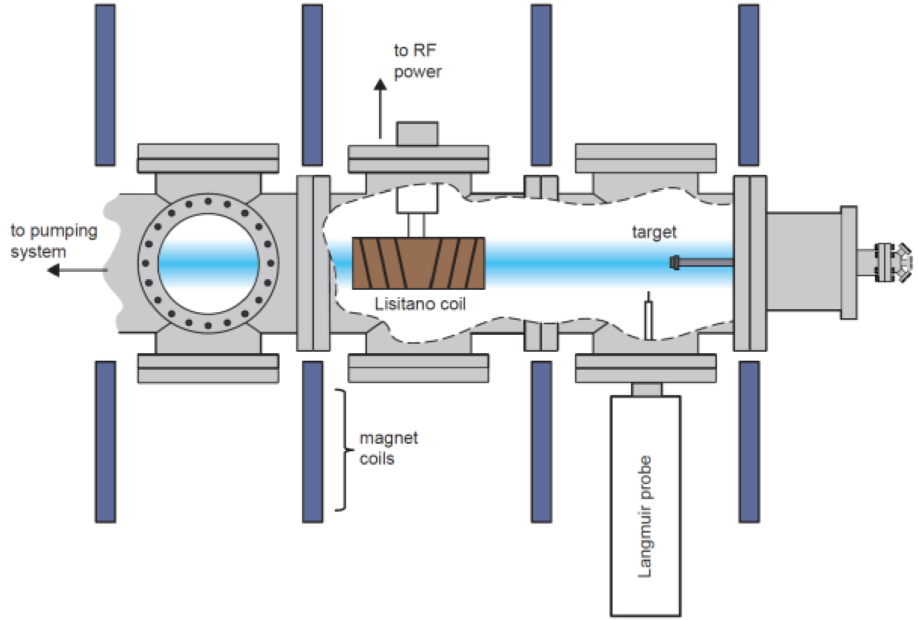
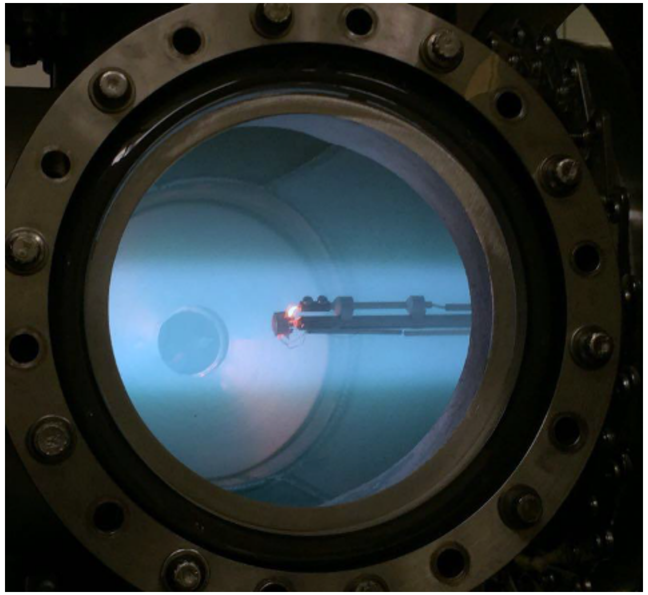
Summary

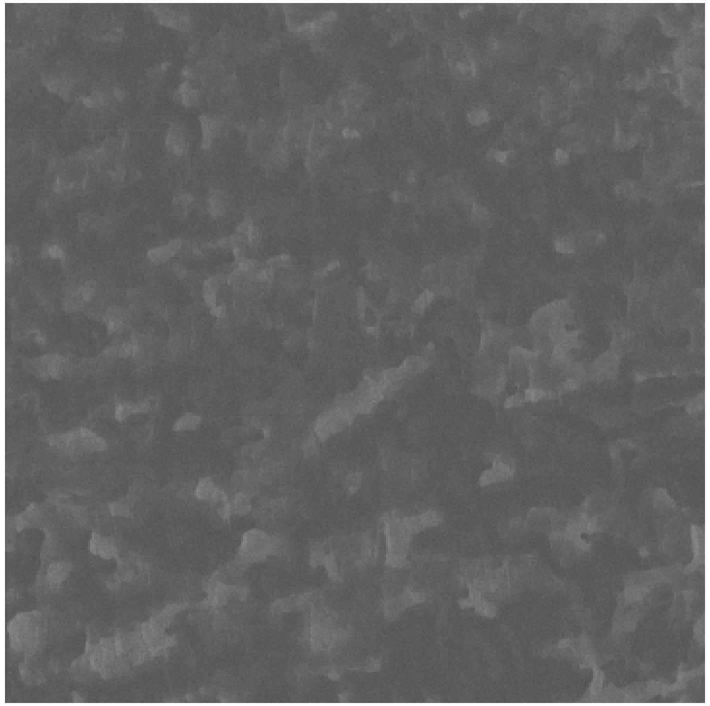
Helium effects on tungsten surfaces



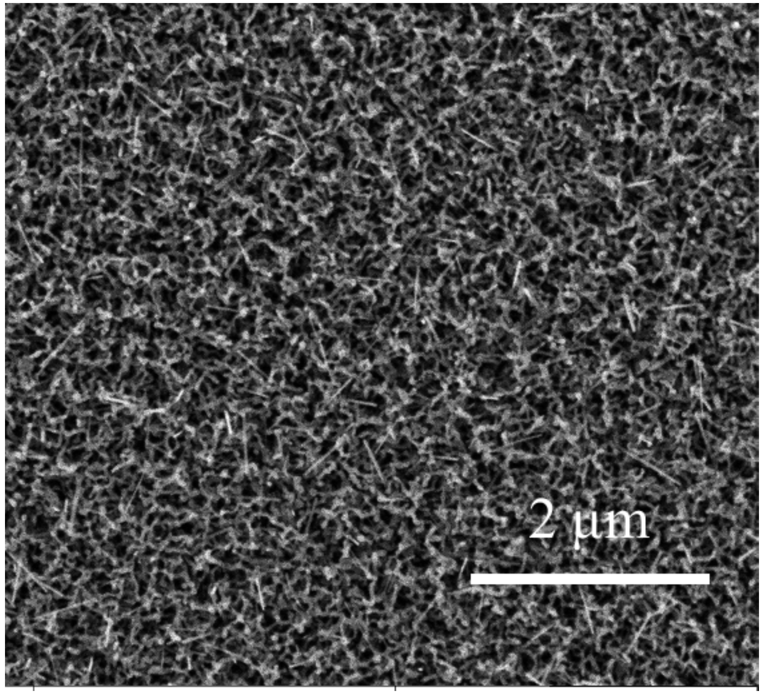


We exposed a tungsten sample to a high-flux helium plasma & imaged surface with helium ion microscopy

Before

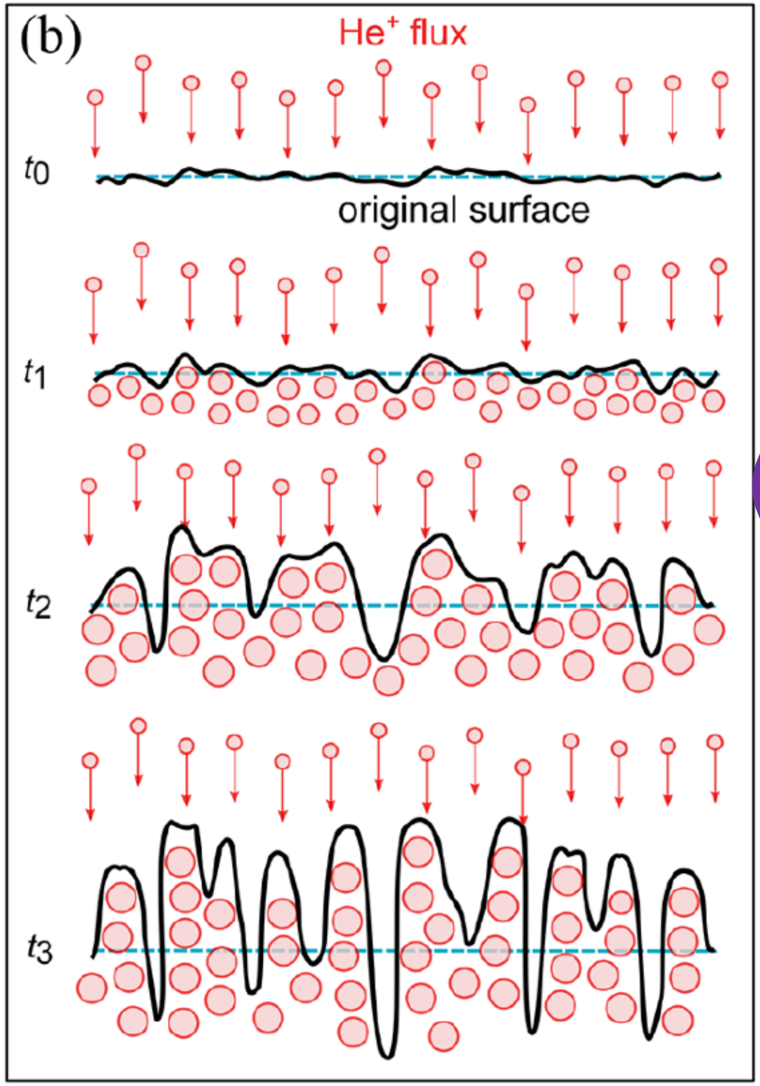


After



the sample had grown “tungsten fuzz”, an effect first discovered by Baldwin and Doerner in 2008

He-induced nanostructure growth on W surfaces



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

- physics for fuzz growth not fully 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

How are the initial defects nucleated and how do these defects grow?

Defects in plasma facing materials

We would like to investigate early stages of defect nucleation and growth due to helium plasma exposure in surface of tungsten

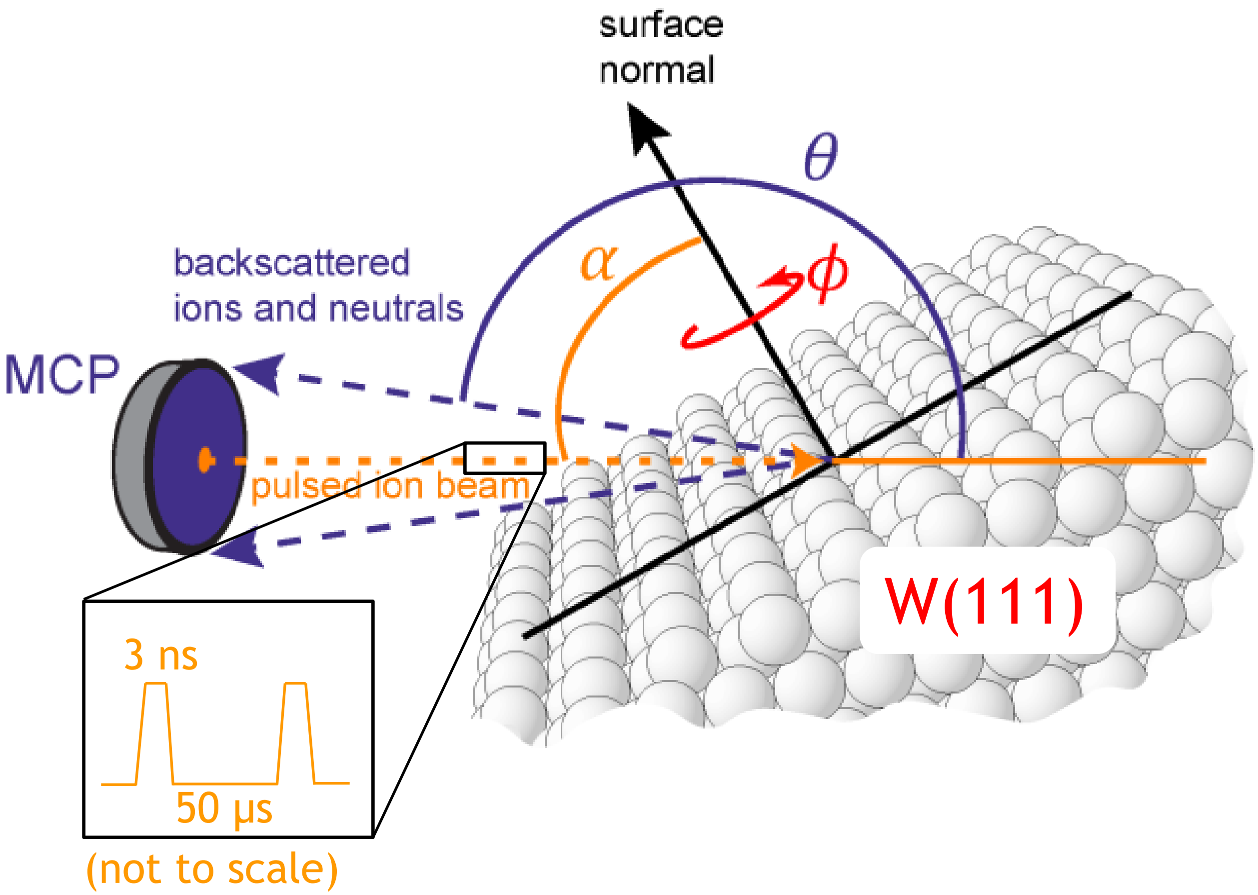
Need to develop: surface science technique sensitive to defect nucleation and growth

1. Capable of detecting atomic-scale changes to surface structure
2. Allow for quantitative comparisons to simulations to interpret data
3. Ideally, suitable for measurements during plasma exposure

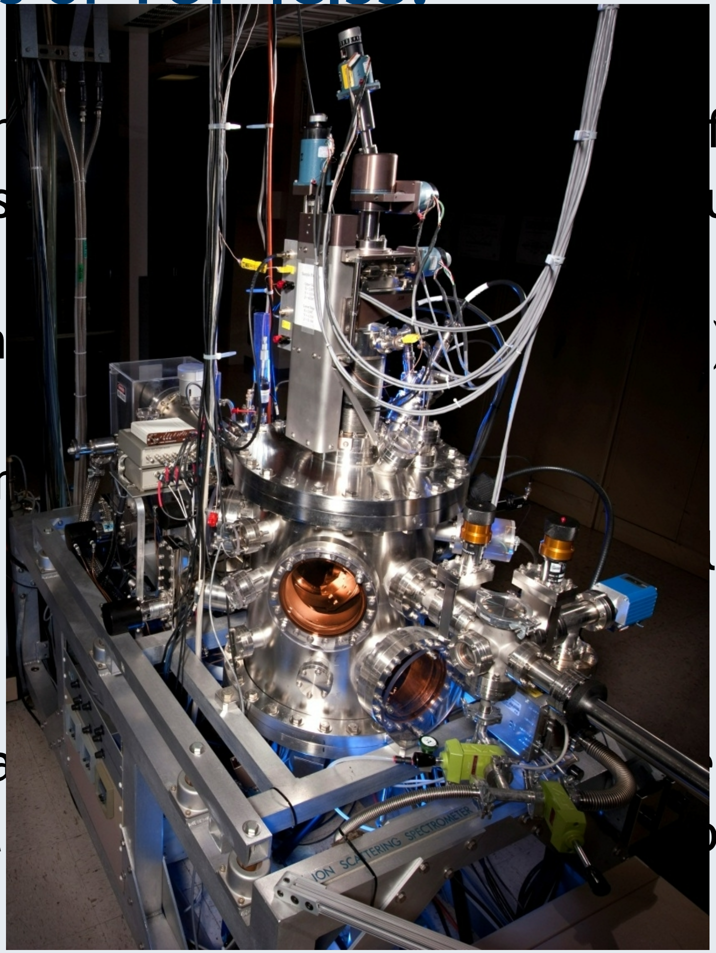
To start: a proof-of-concept characterization of a pristine W(111) surface structure using impact-collision ion scattering spectroscopy (ICISS)

TOF-ICISS

Time-of-flight impact-collision ion scattering spectroscopy

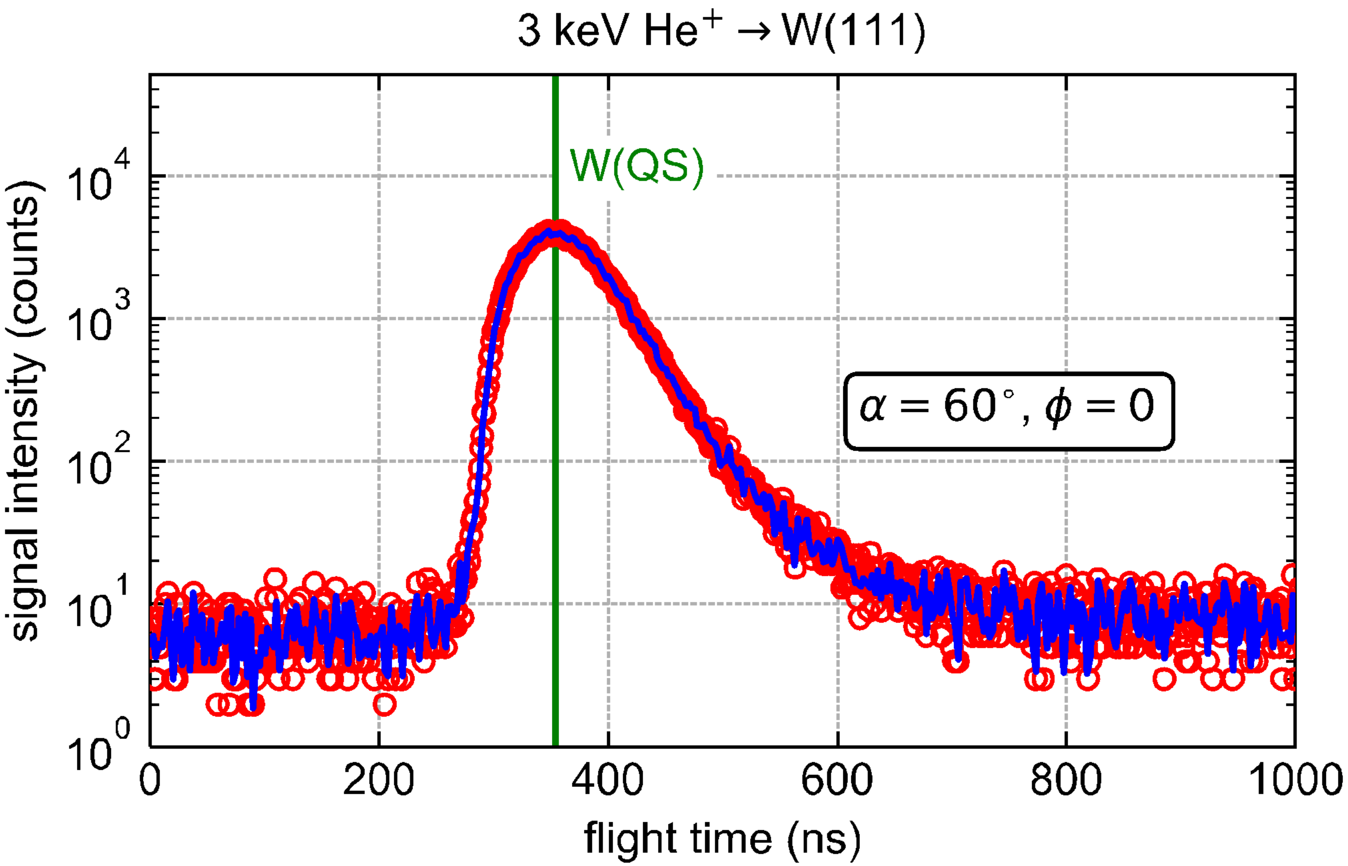


Strengths of TOF-ICISS:



- Ser … f the
  firs … urface
- Ion …)
- Sim … LEIS:
  - … llisions
  - …
- Tra … d by
  EM … ons

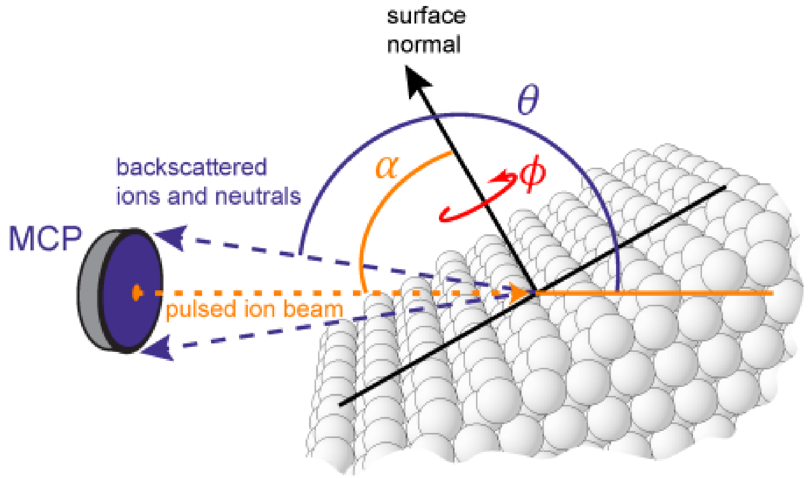
Representative time-of-flight spectrum

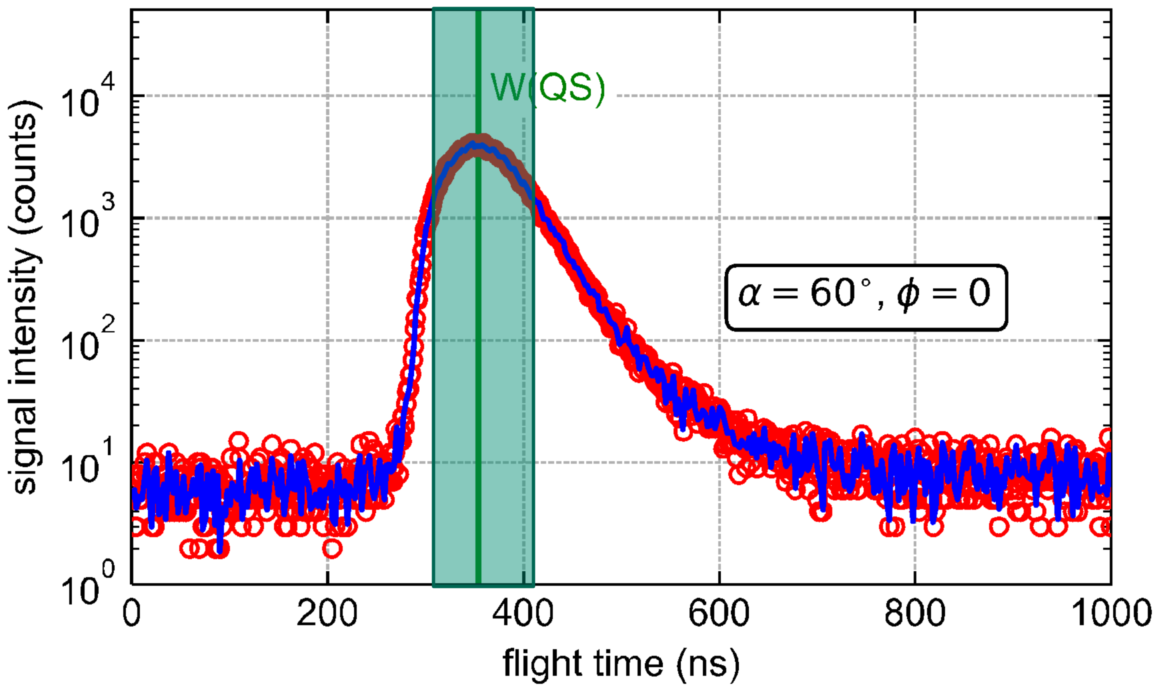


higher energy
fewer collisions before backscattering

lower energy
more collisions before backscattering

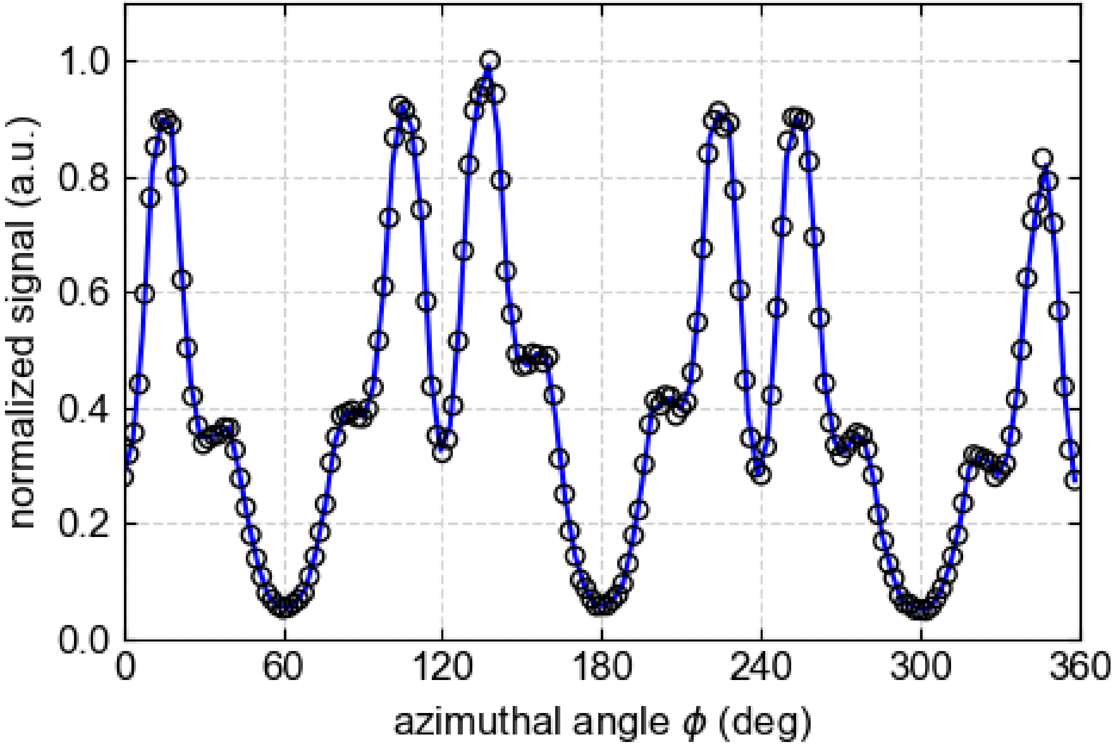
How does the signal vary with crystalline orientation?



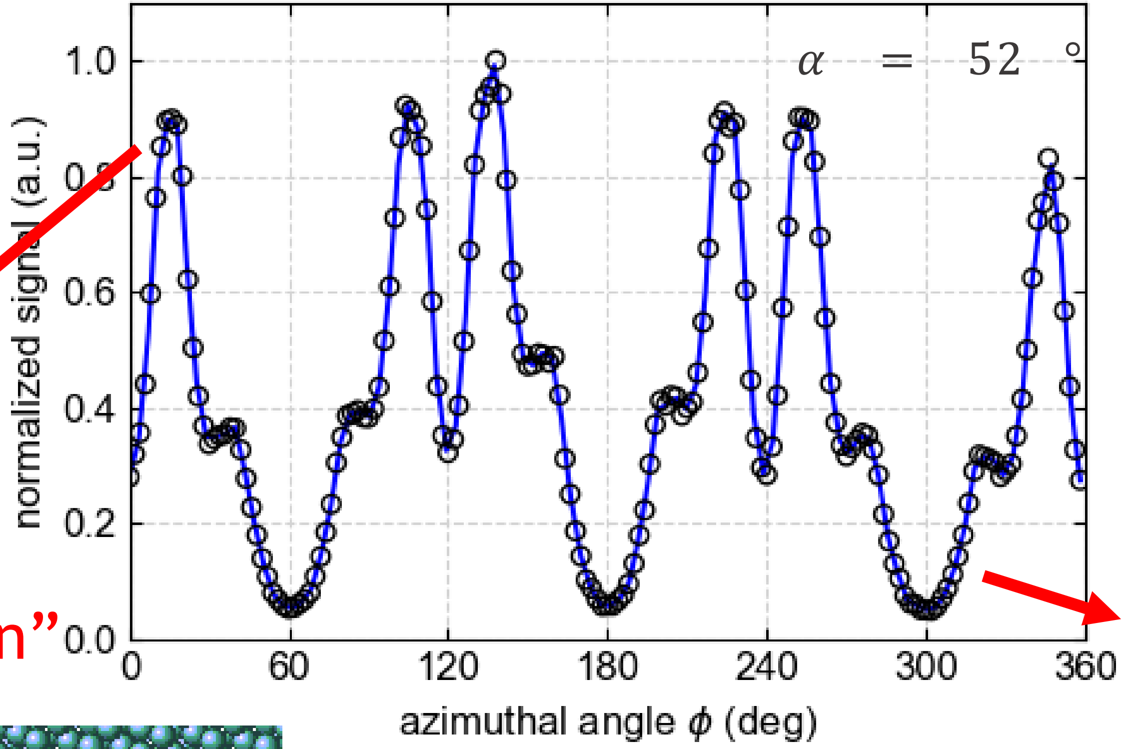


Azimuthal rotation (ϕ)

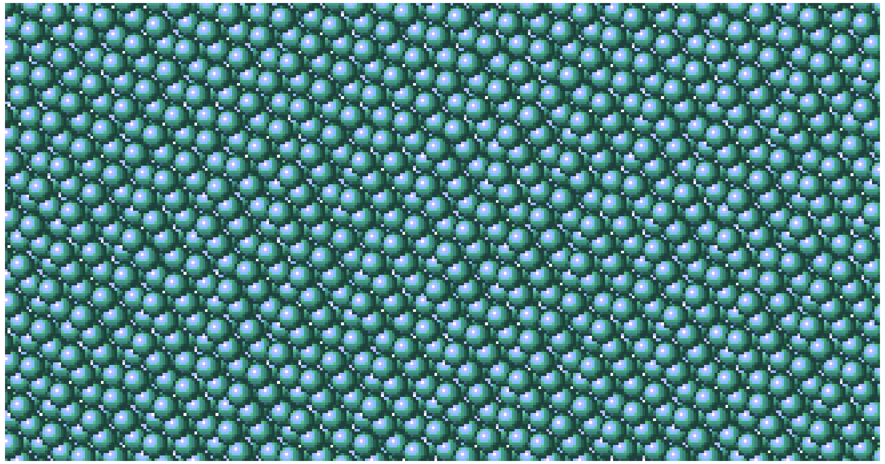
$\alpha = 52°$



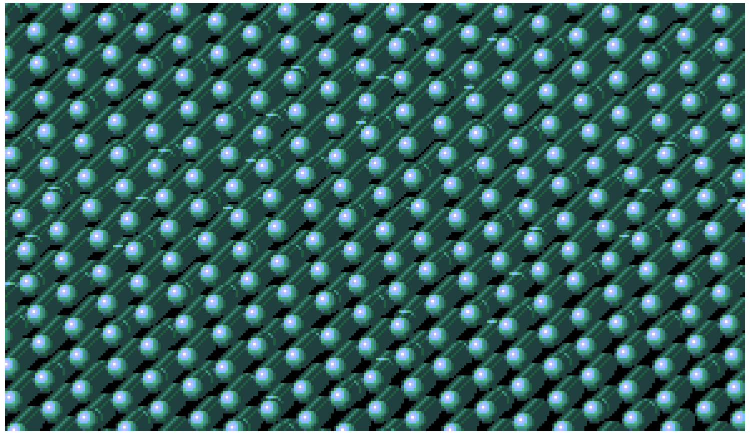
He$^+$ channeling (simplified picture)



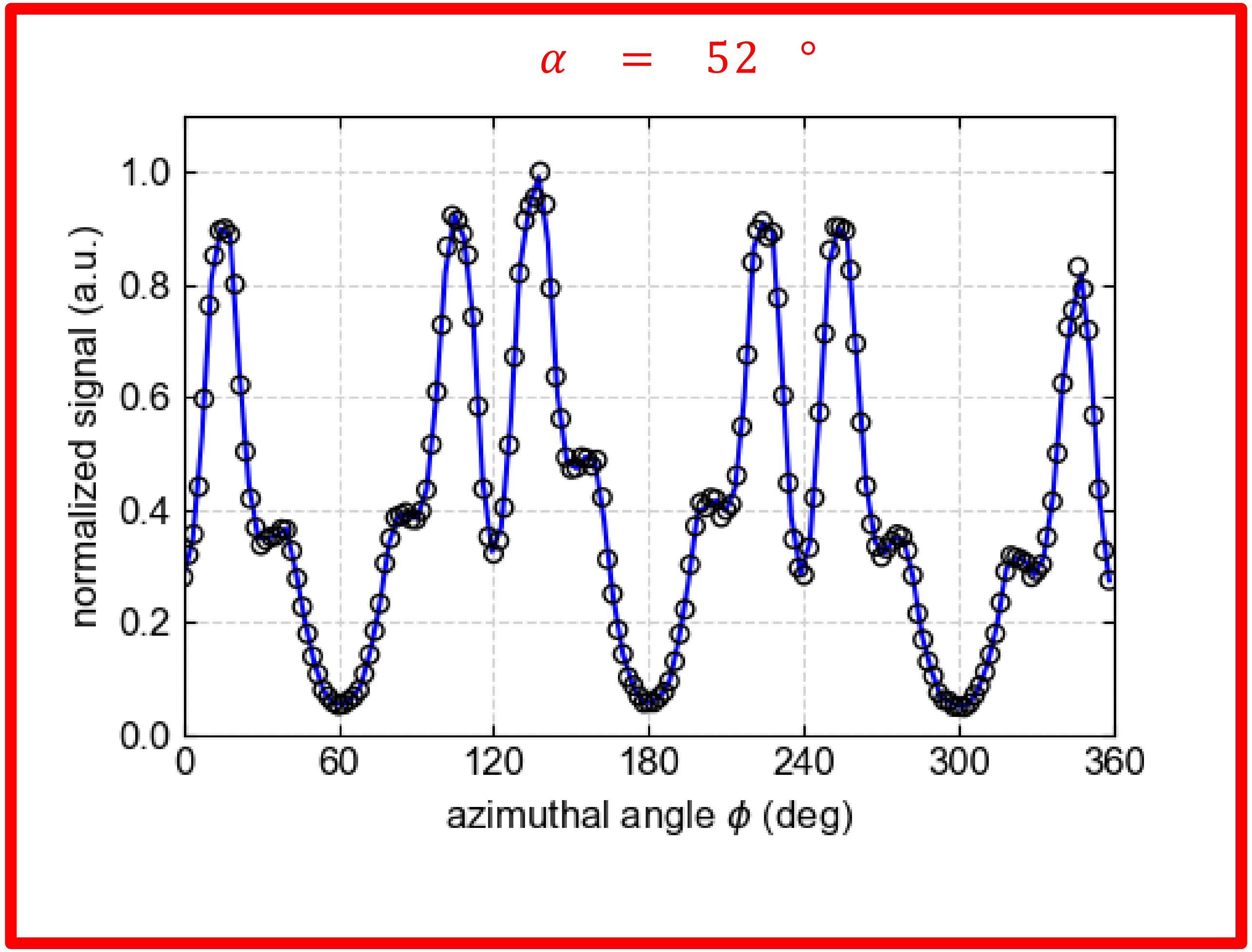
Large signal:
"random orientation"

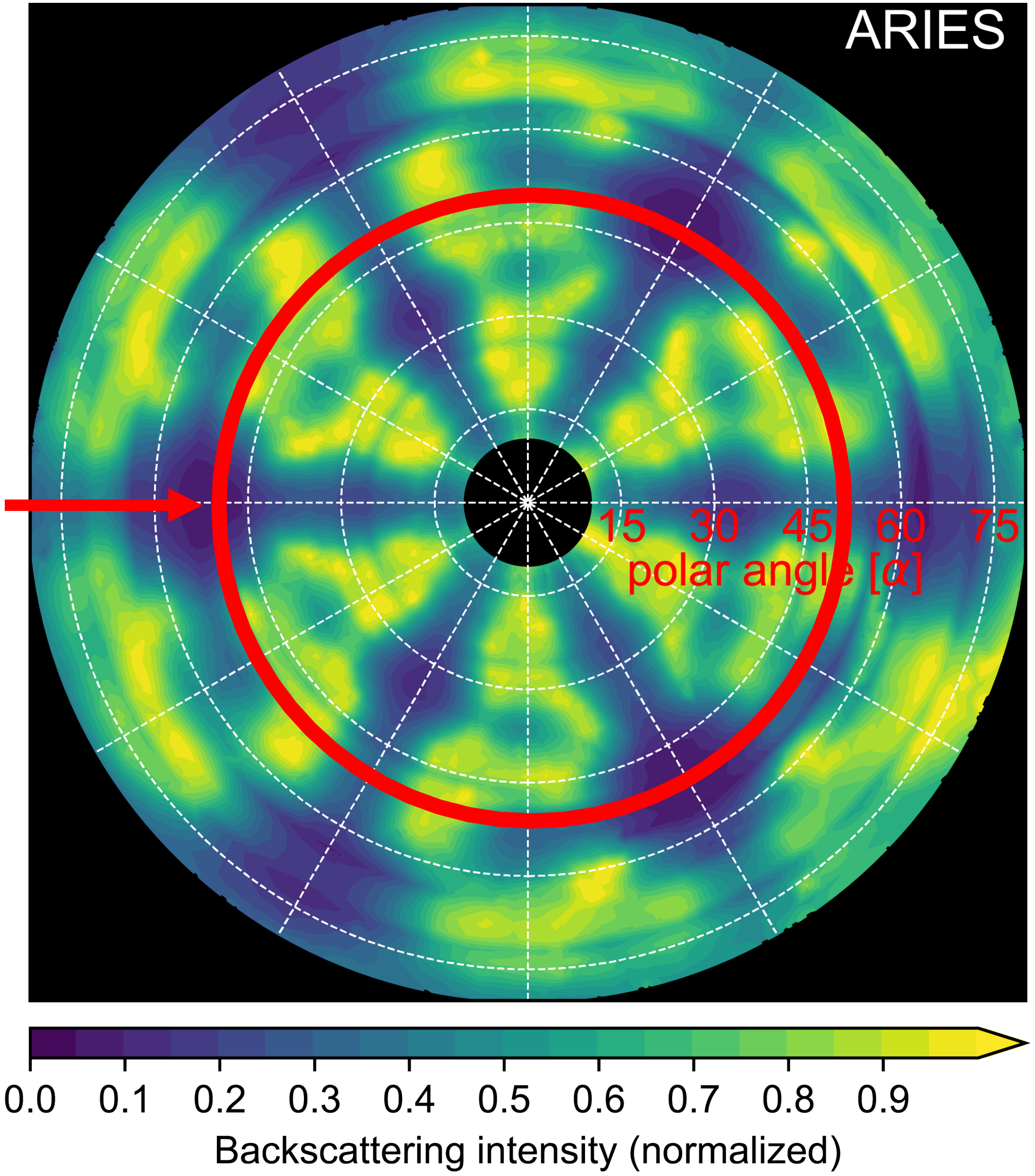


Small signal:
subsurface atoms aligned

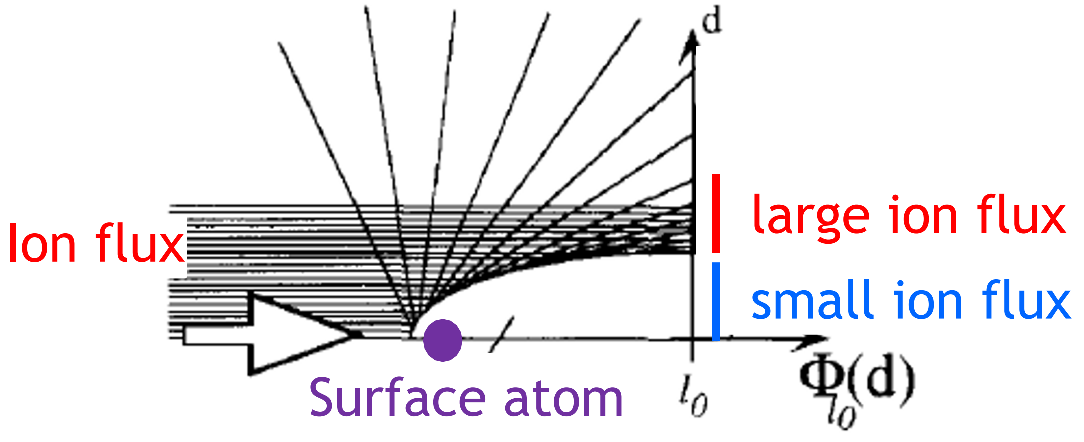


Generating multi-angle maps

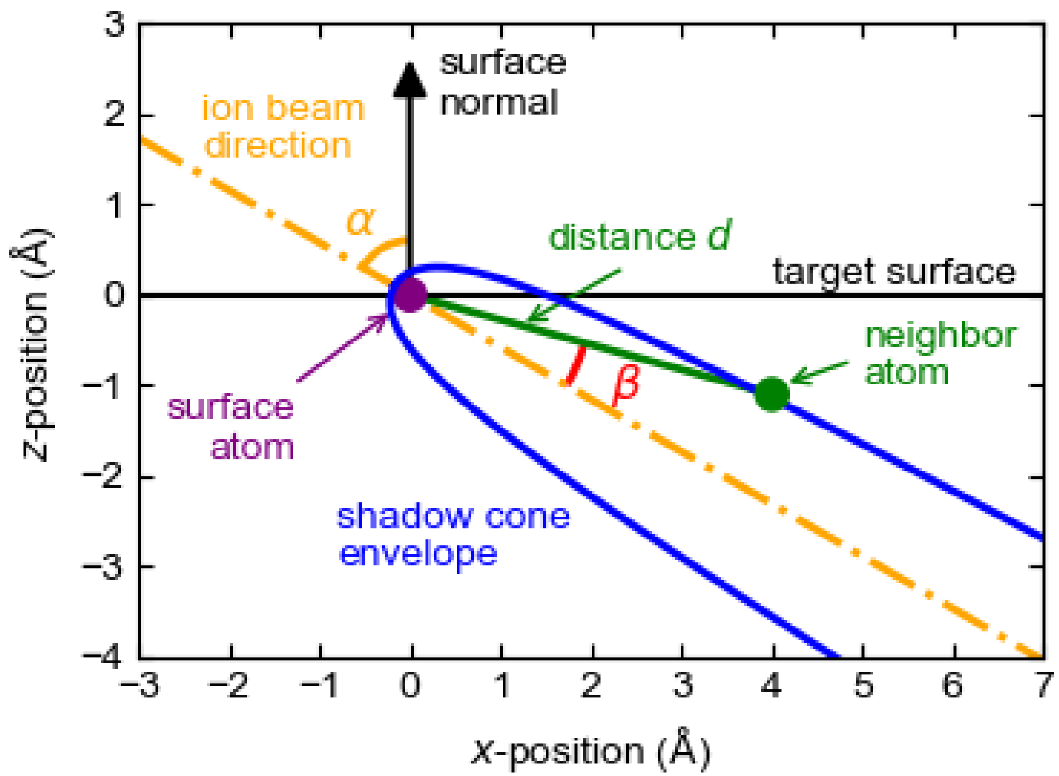




Shadow cones

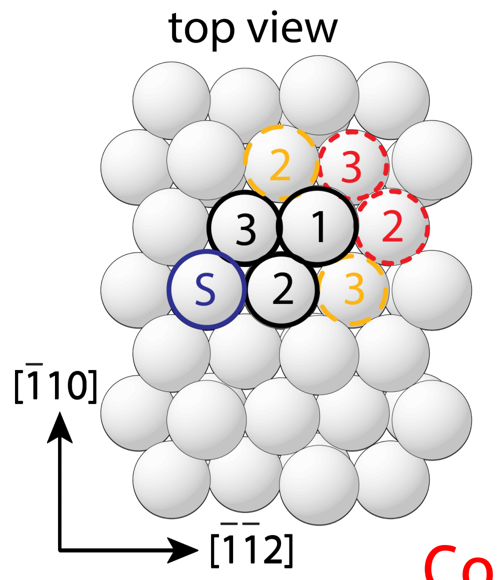


Agostino et al., Surf. Sci. **384,** (1997).

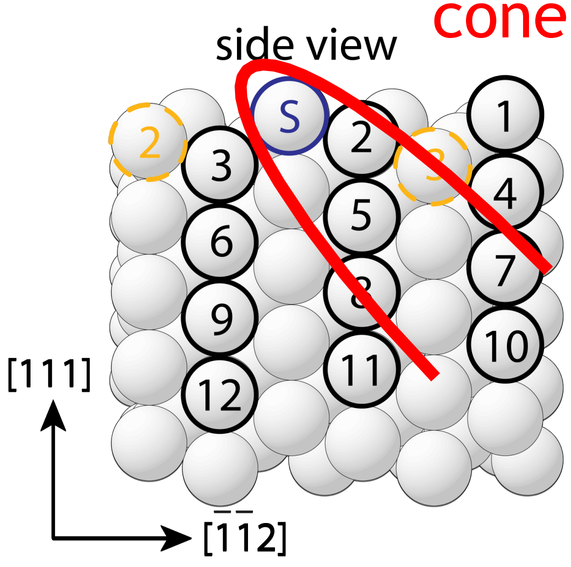


- Shadow cone arises from ion focusing
- Enhanced signal when cone coincides with neighboring atom; reduced signal when neighbor is within cone

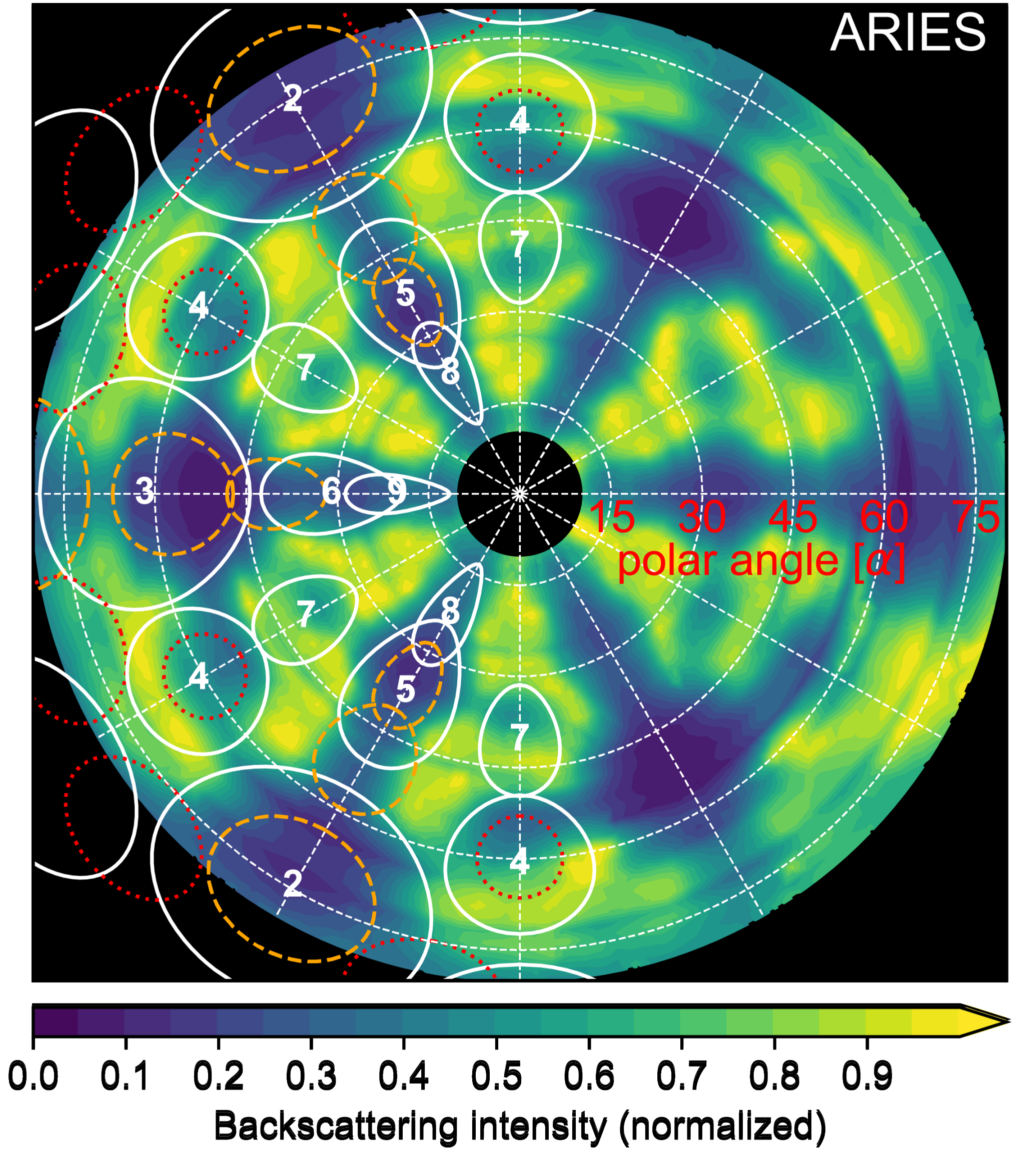
Shadow-cone analysis of multi-angle maps



Compute angles when cone intercepts neighbors



Plot the computed shadow cone angles—"shadow lines"

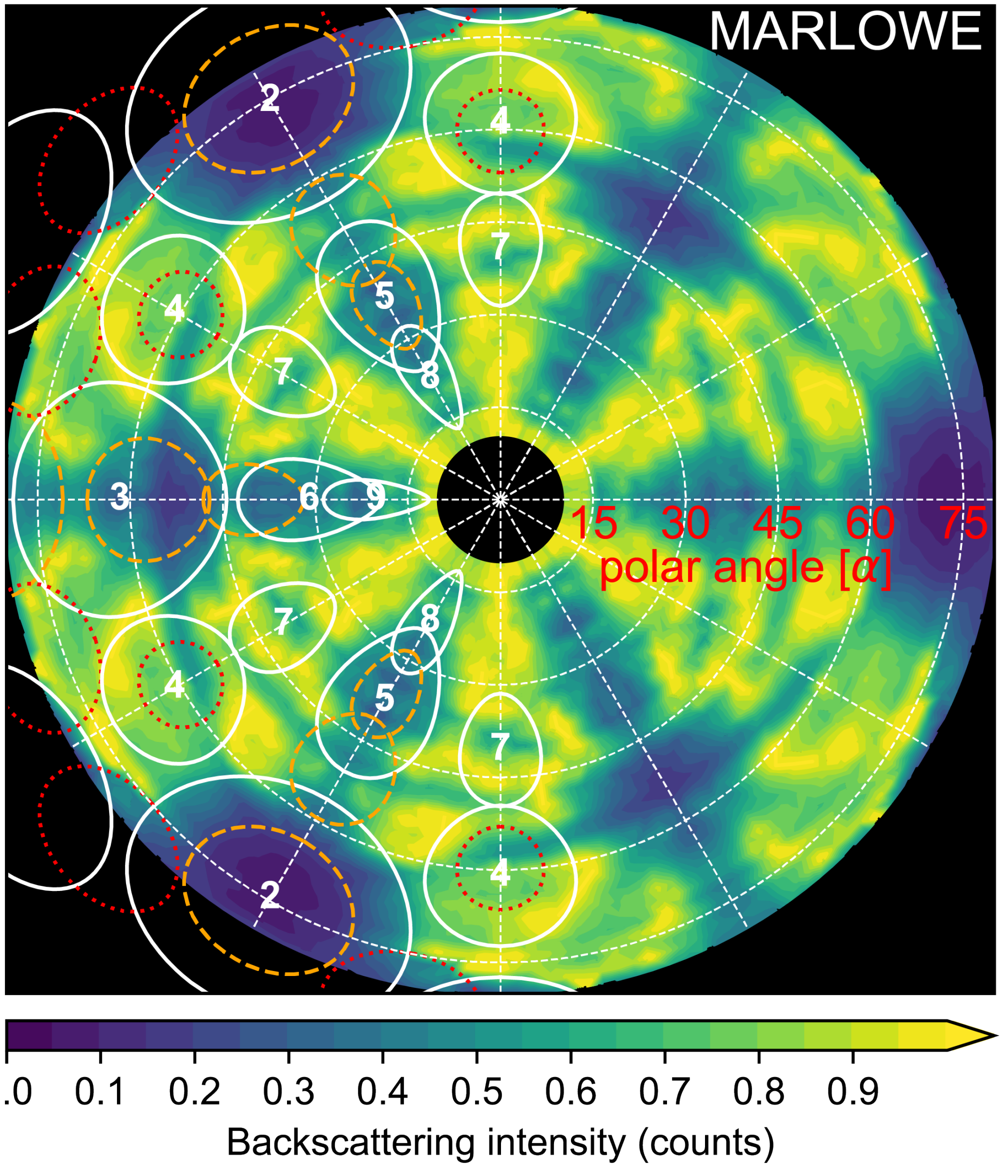


Modeling: MARLOWE

MARLOWE map simulation

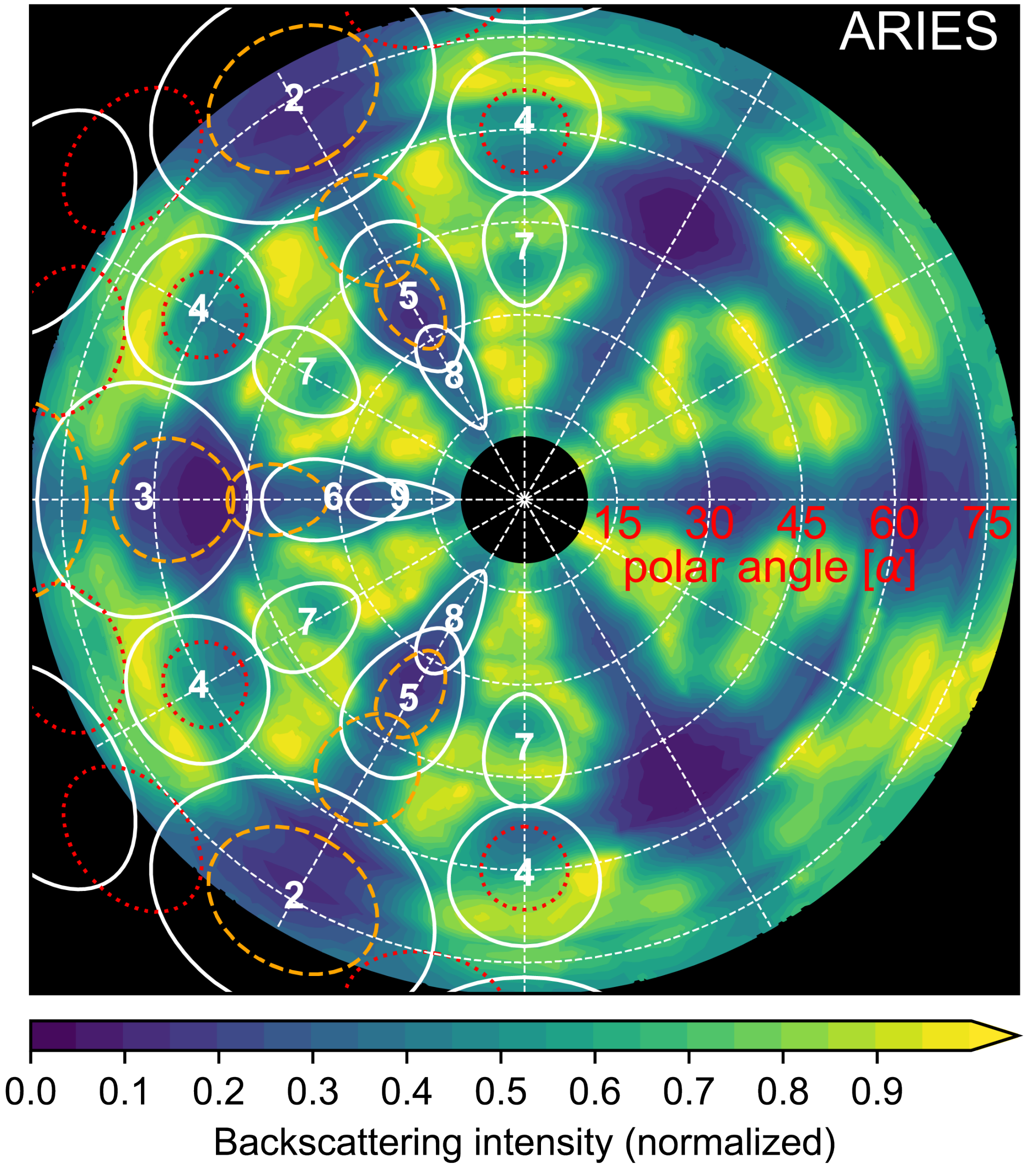
- Binary collision approximation
  - Faster than molecular dynamics
  - Collisions assume ZBL potential
  - Fails for multi-body collisions
- 2 million incident ions for each (α,ϕ), surface reset between each ion
- Data analyzed in the same way as in experiment

Simulation

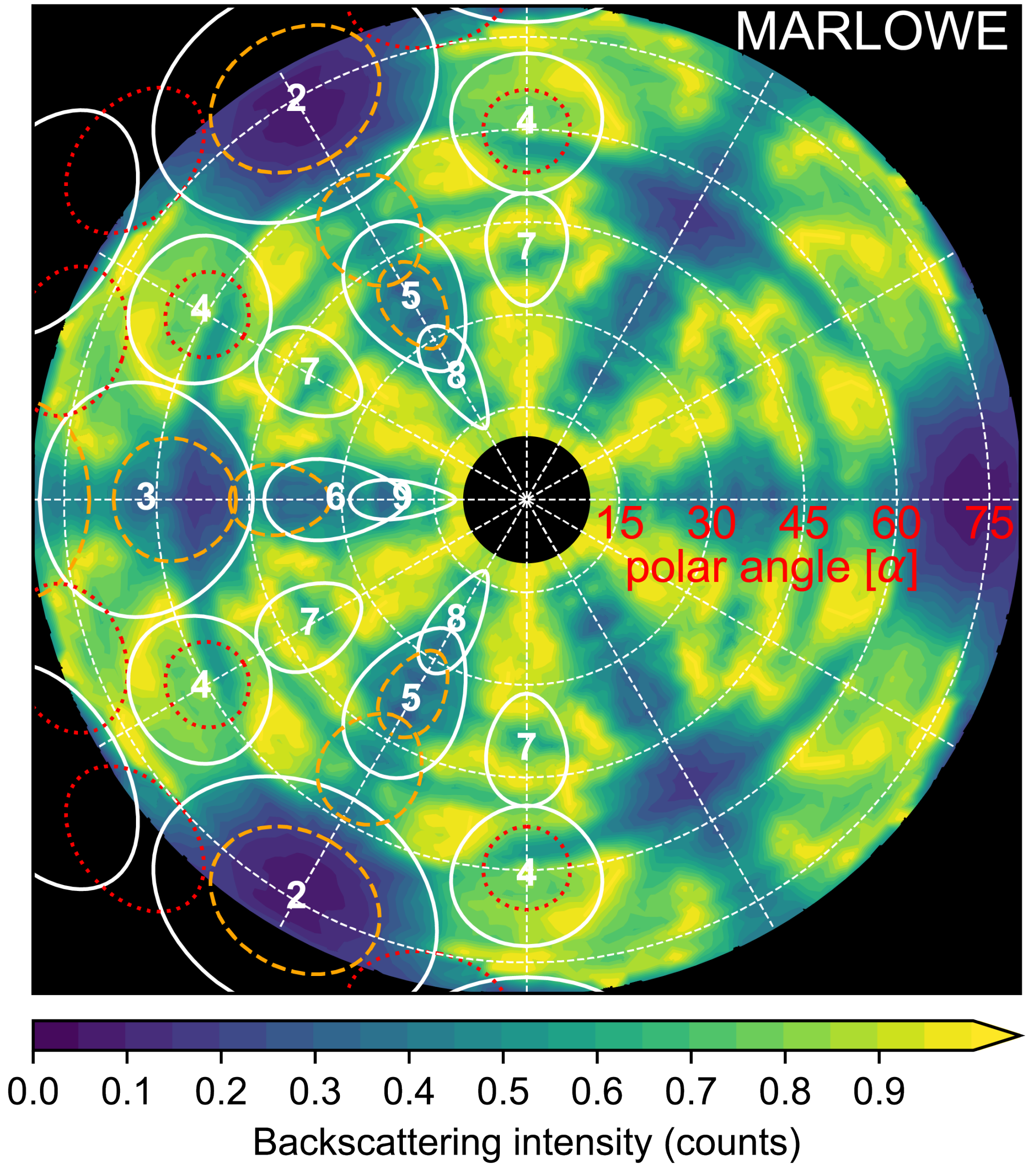


Modeling: MARLOWE

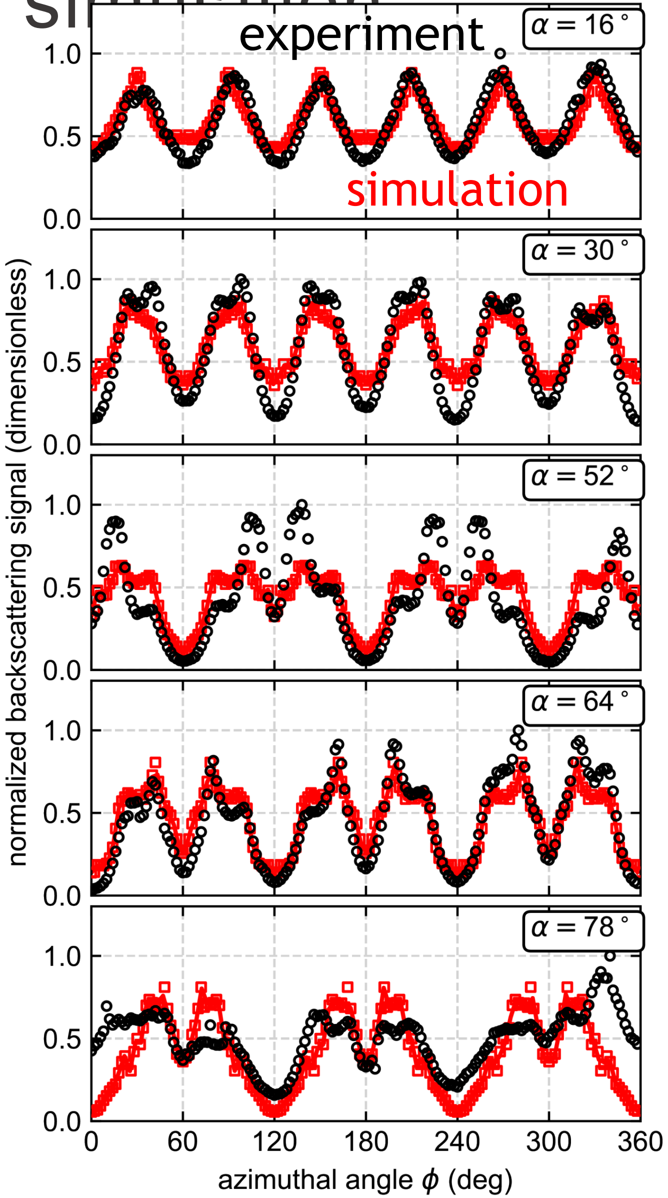
Experiment



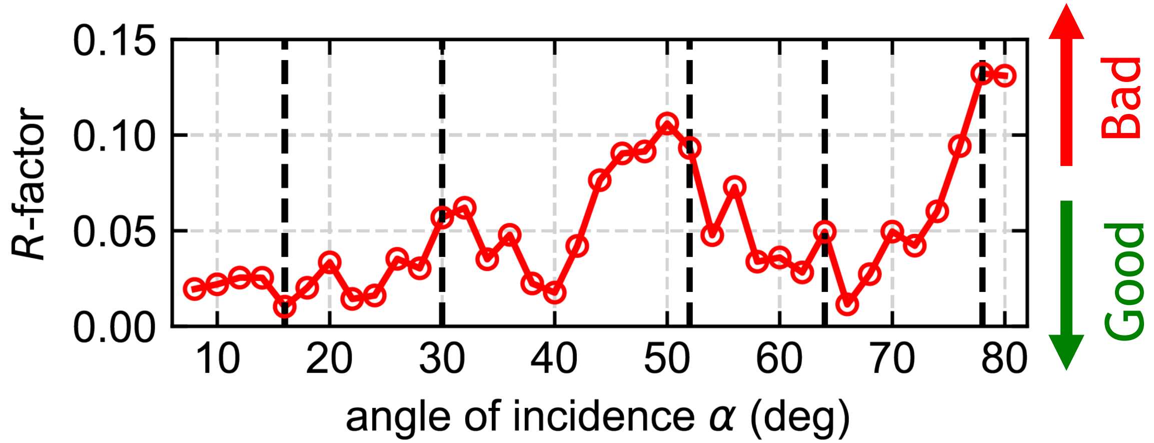
Simulation



Quantitative comparison between experiment and simulation



R-factor
(least squares fit)



Experiment & simulation allow for quantitative comparisons

ICISS + modeling will be used to quantitatively investigate initial helium-induced defect formation and growth

Outline

Fusion energy & materials challenges

- What is fusion and how does it work?
- What are key materials issues that need to be addressed?

Low energy ion beam analysis of material surfaces

- Hydrogen adsorption on tungsten(111)
- Structural studies of tungsten(111) to understand defect nucleation & growth
- **Ongoing/future work**
  - Impurity effects on hydrogen adsorption on tungsten surfaces
  - Characterization of more complex surface structures

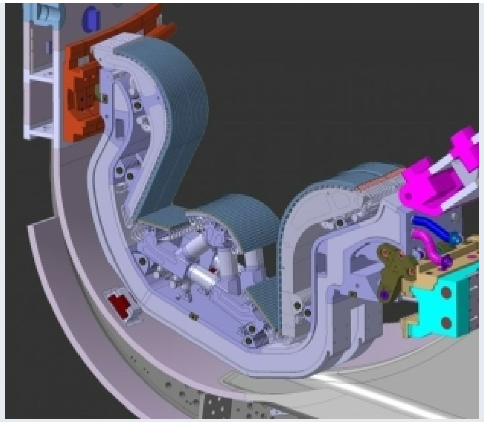
Summary

Nitrogen interactions with tungsten

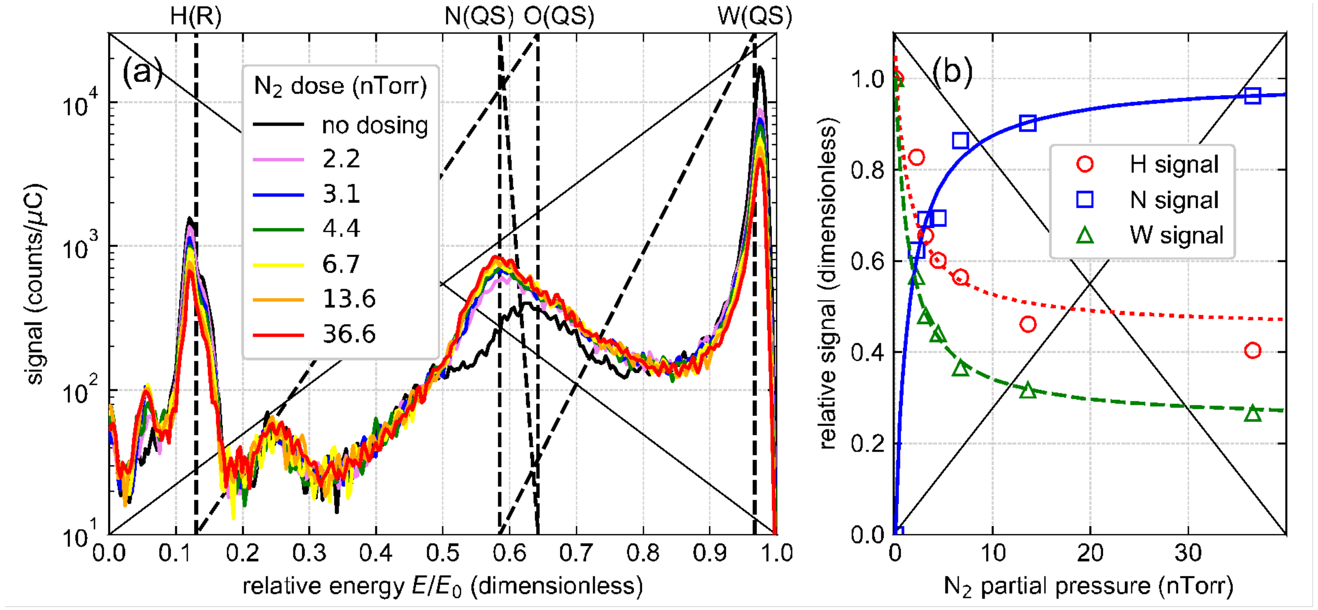
Nitrogen will be introduced into divertor to lessen heat load on surfaces:

- How does N interact with W surfaces?
- How does this impact H adsorption?

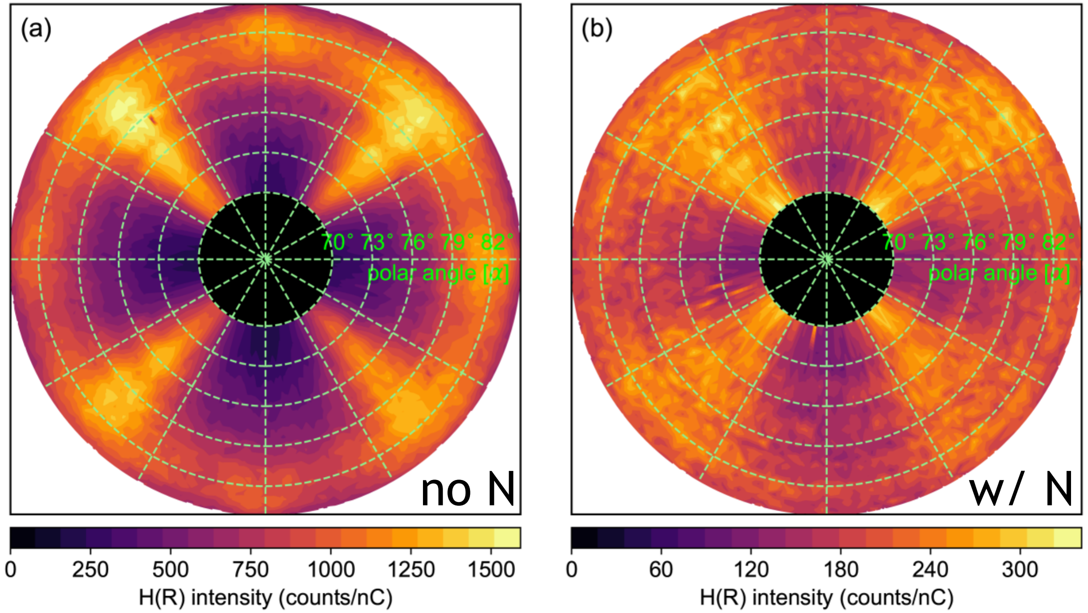
Dose W surface with N_2 during LEIS + DRS measurements



Polycrystalline tungsten



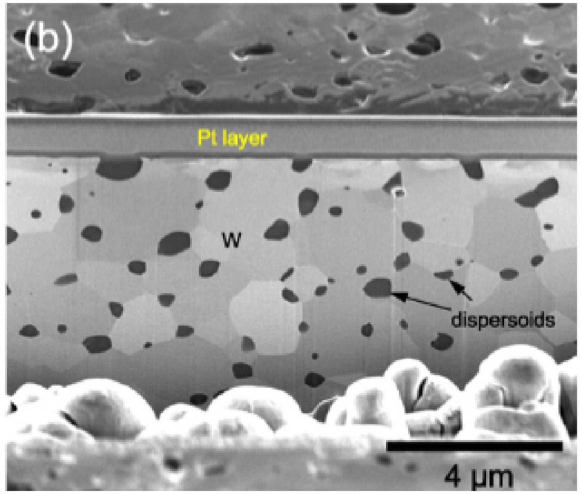
Tungsten single crystal W(100)



We observe reduction in H by presence of N on surface

More complex, multi-component crystalline materials

UFG-W (Ti dispersoids)



Kolasinski et al., IJRMHM, (2016).

Pure tungsten is likely insufficient for a fusion power plant

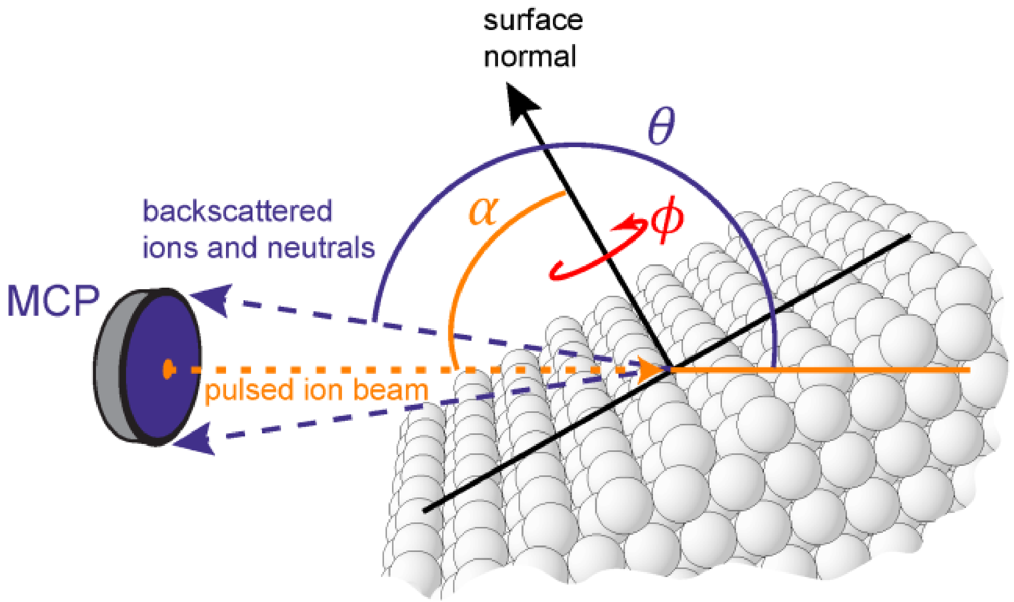
- High temperatures, leading to recrystallization & melting
- Neutron damage

Alternatives include advanced tungsten materials

- Tungsten alloys
- Dispersoids in tungsten

We would like to characterize more complex surface structures with ICISS:

- fewer symmetries
- more components

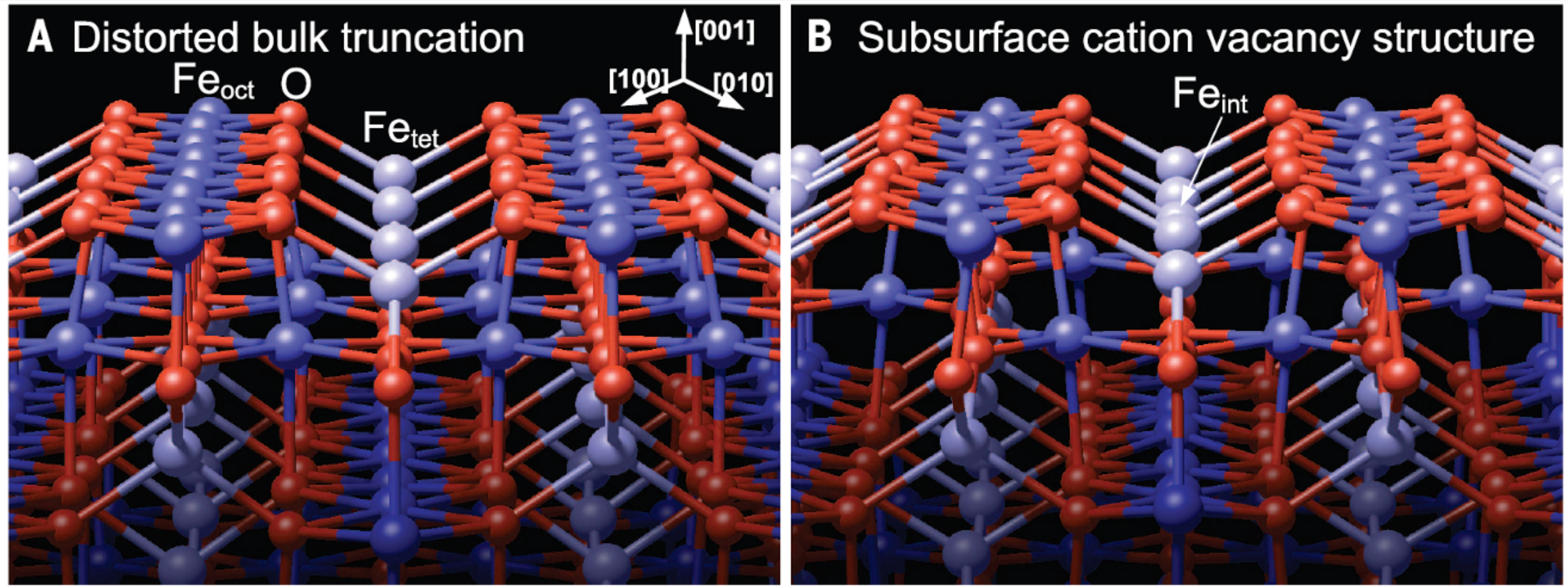


Characterizing surface structure of a metal oxide, Fe_3O_4

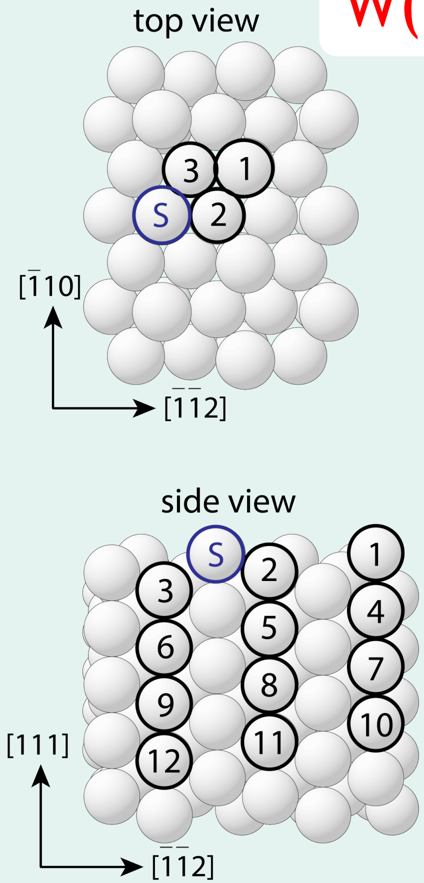
Surface structure of $Fe_3O_4(100)$ is much more complex than W(111)!

DB: Pentcheva et al. PRL 2005

SCV: Bliem et al. Science 2014

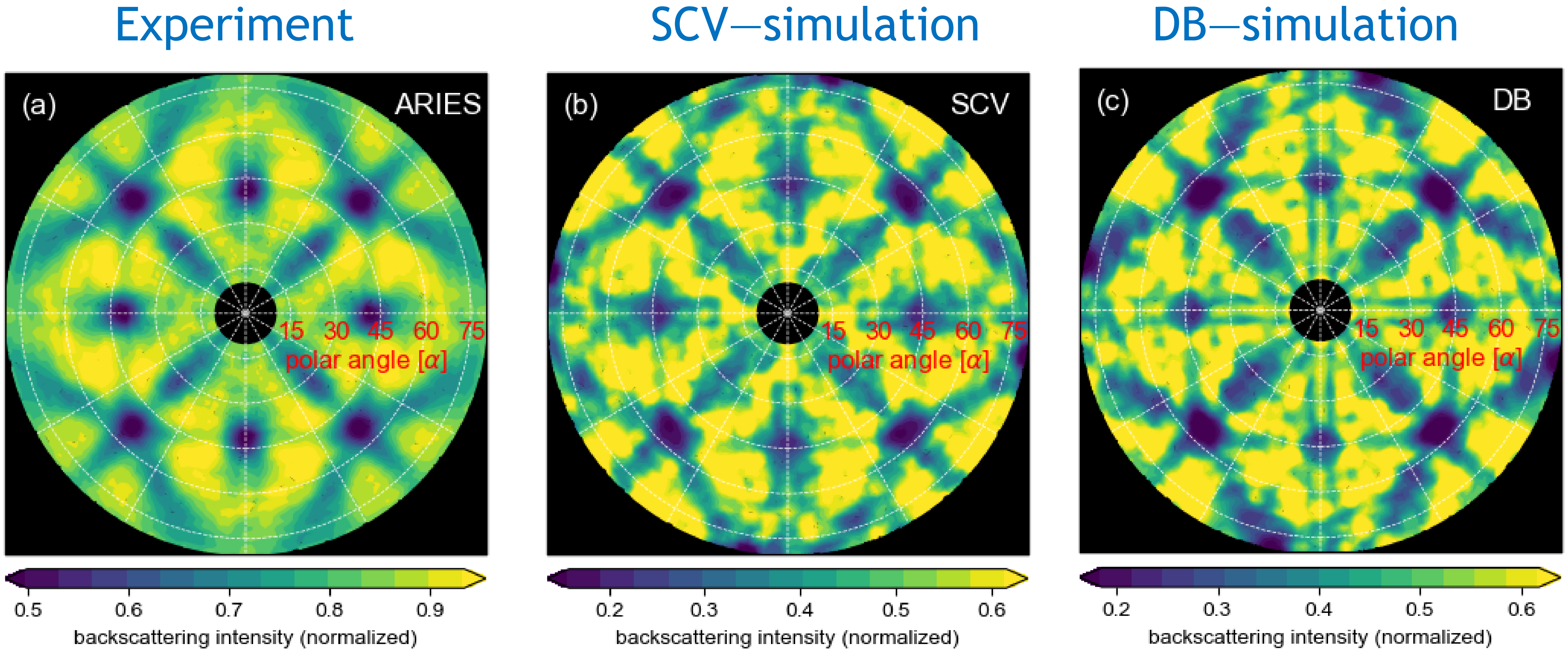


W(111)



$Fe_3O_4(100)$ serves as a model surface—to what extent can we differentiate between the two surface structures with ICISS?

ICISS of $Fe_3O_4(100)$



SCV model provides better qualitative agreement with experiment: further work needed to achieve quantitative agreement

Summary

Hydrogen adsorption sites on W(111)

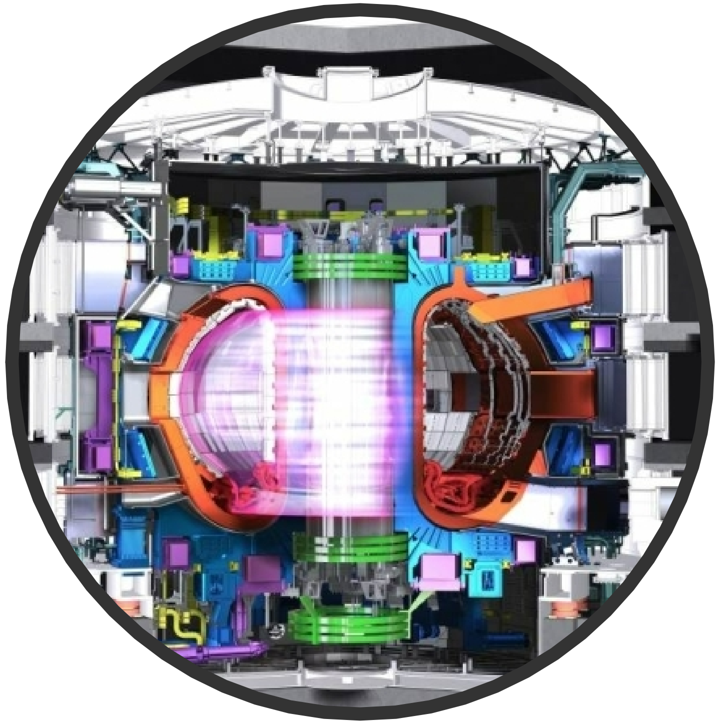
- LEIS + DRS multi-angle mapping W and H signals
- MD simulations to identify precise H locations

Surface structure of W(111) to study defects

- Experimental ICISS mapping of W signal
- BCA modeling with quantitative comparisons to experiment

Ongoing/Future work

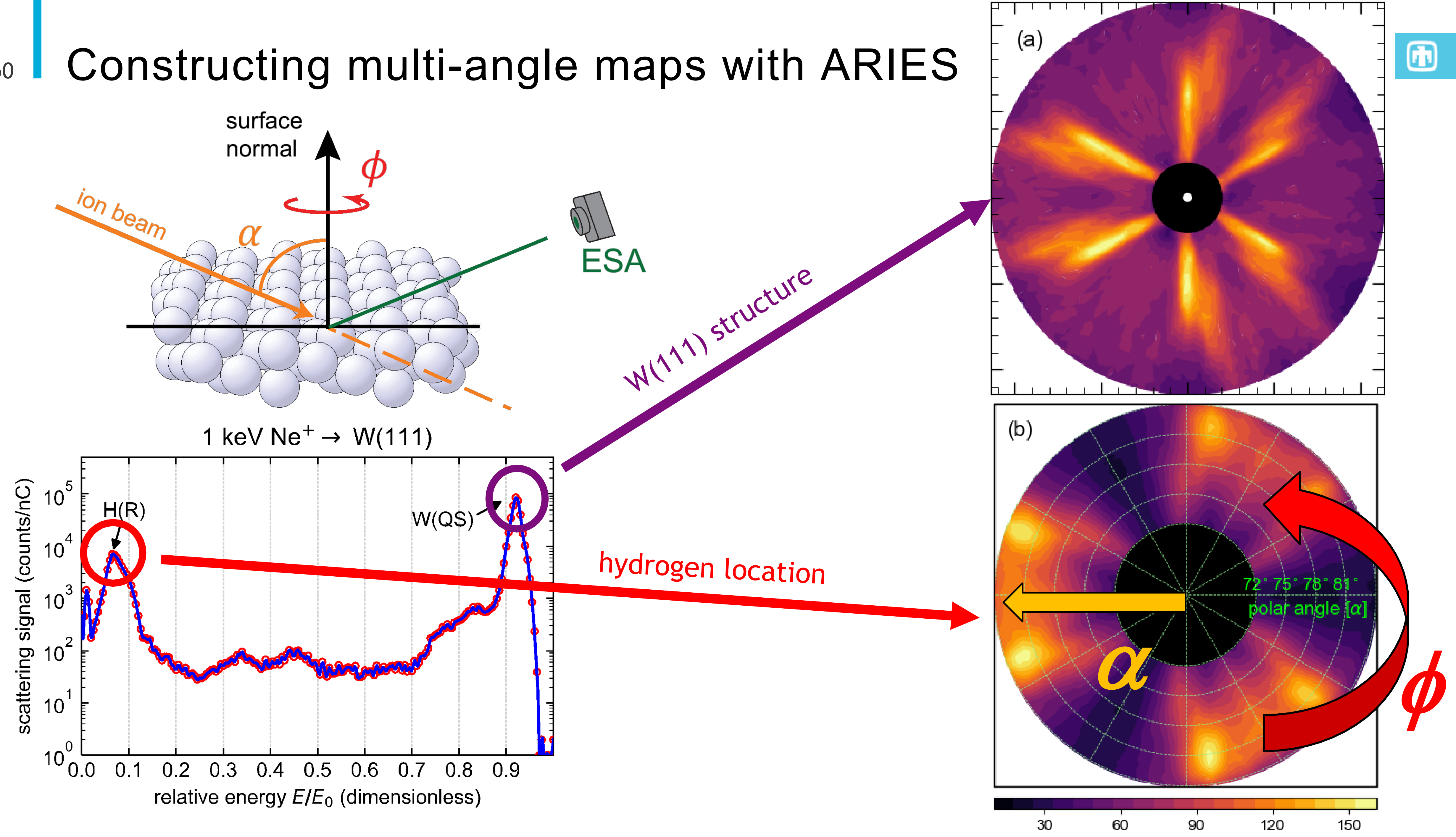
- Effect of impurities on plasma facing surfaces
- Structural studies of more complex materials



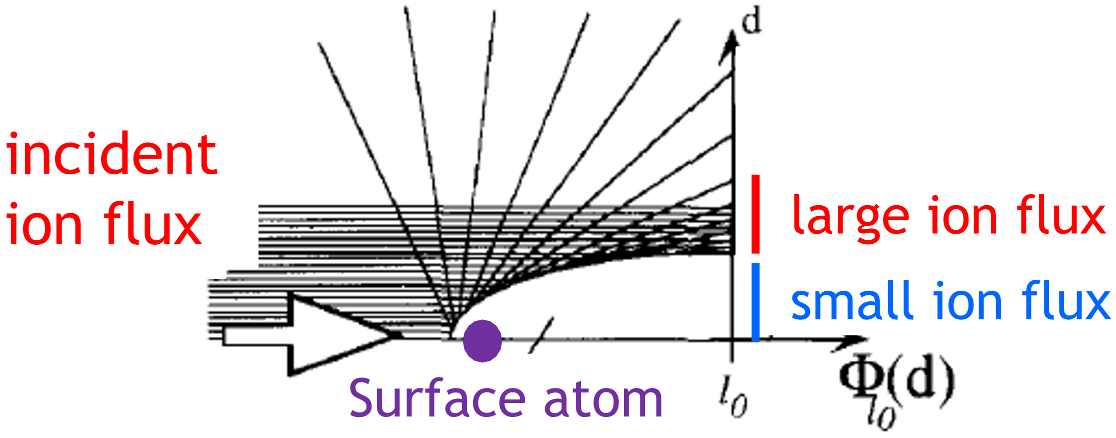
Thank you for your attention!

Extra slides

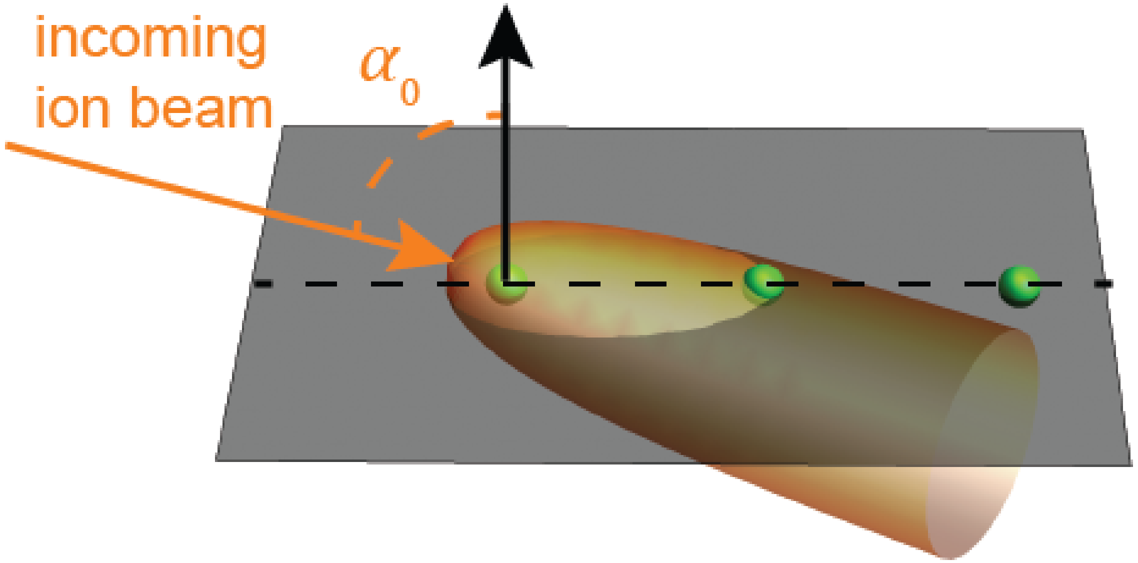
Constructing multi-angle maps with ARIES



Shadow cones

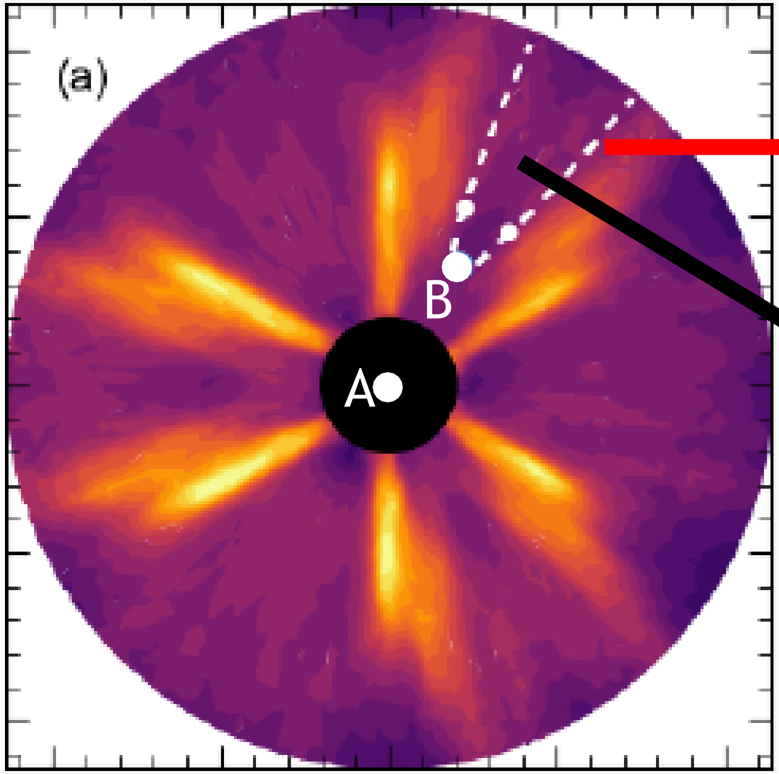


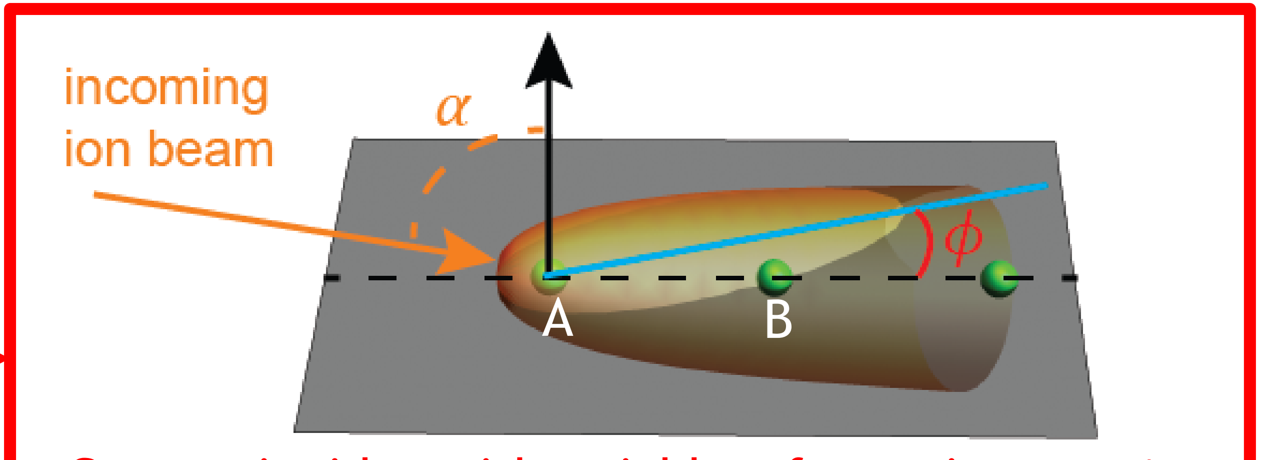
Agostino et al., Surf. Sci. **384,** (1997).



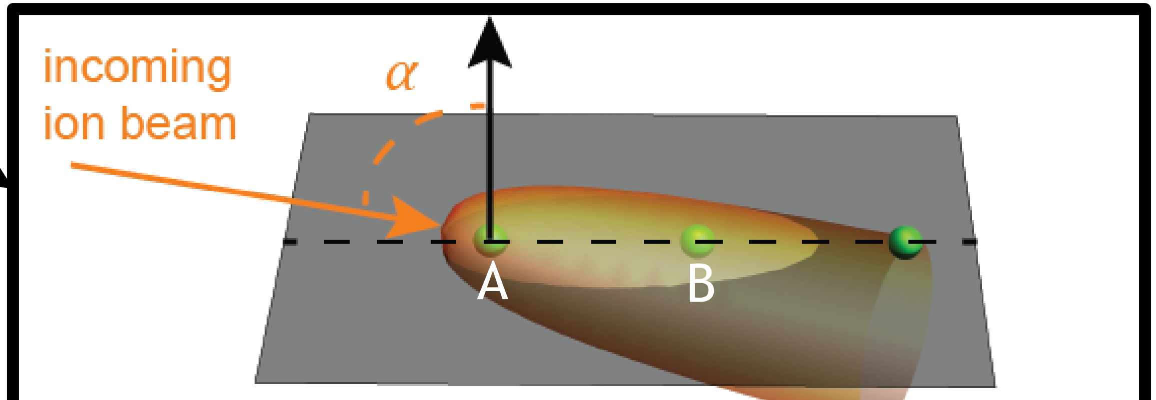
- Shadow cone arises from ion focusing
- Enhanced signal when cone coincides with neighboring atom; reduced signal when neighbor is within cone

Shadow line analysis





Cone coincides with neighbor for various α, ϕ



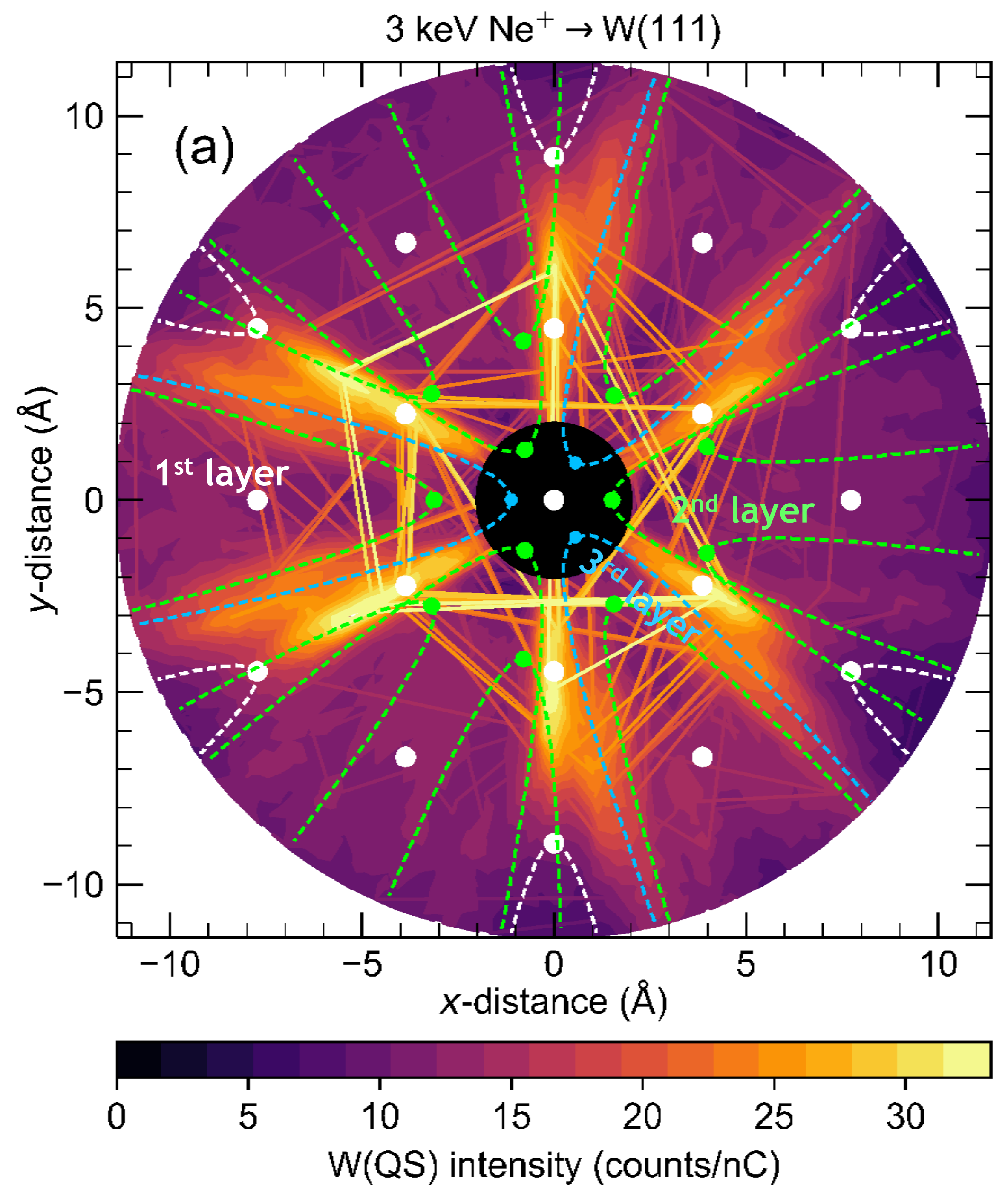
Neighbor inside shadow cone

Shadow line:

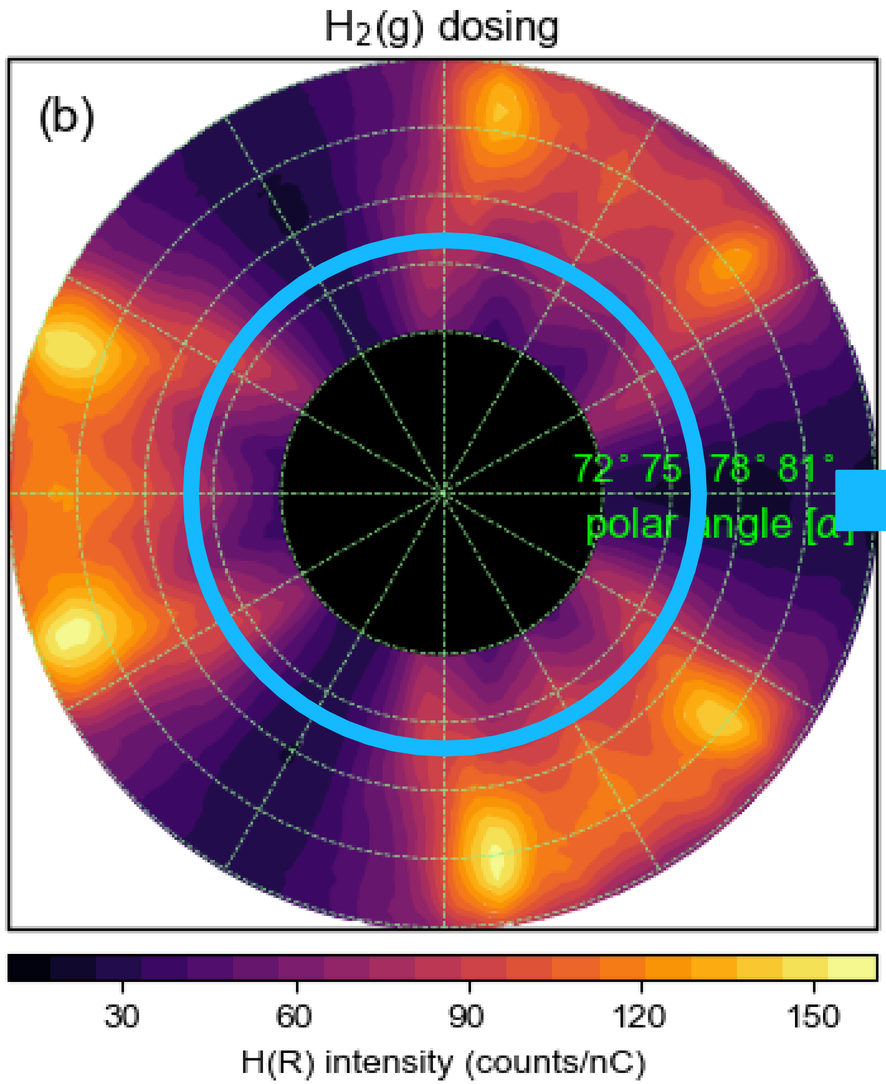
- Traces out α, ϕ that shadow cone coincides with W atom
- delineates region of enhanced scattering from diminished scattering

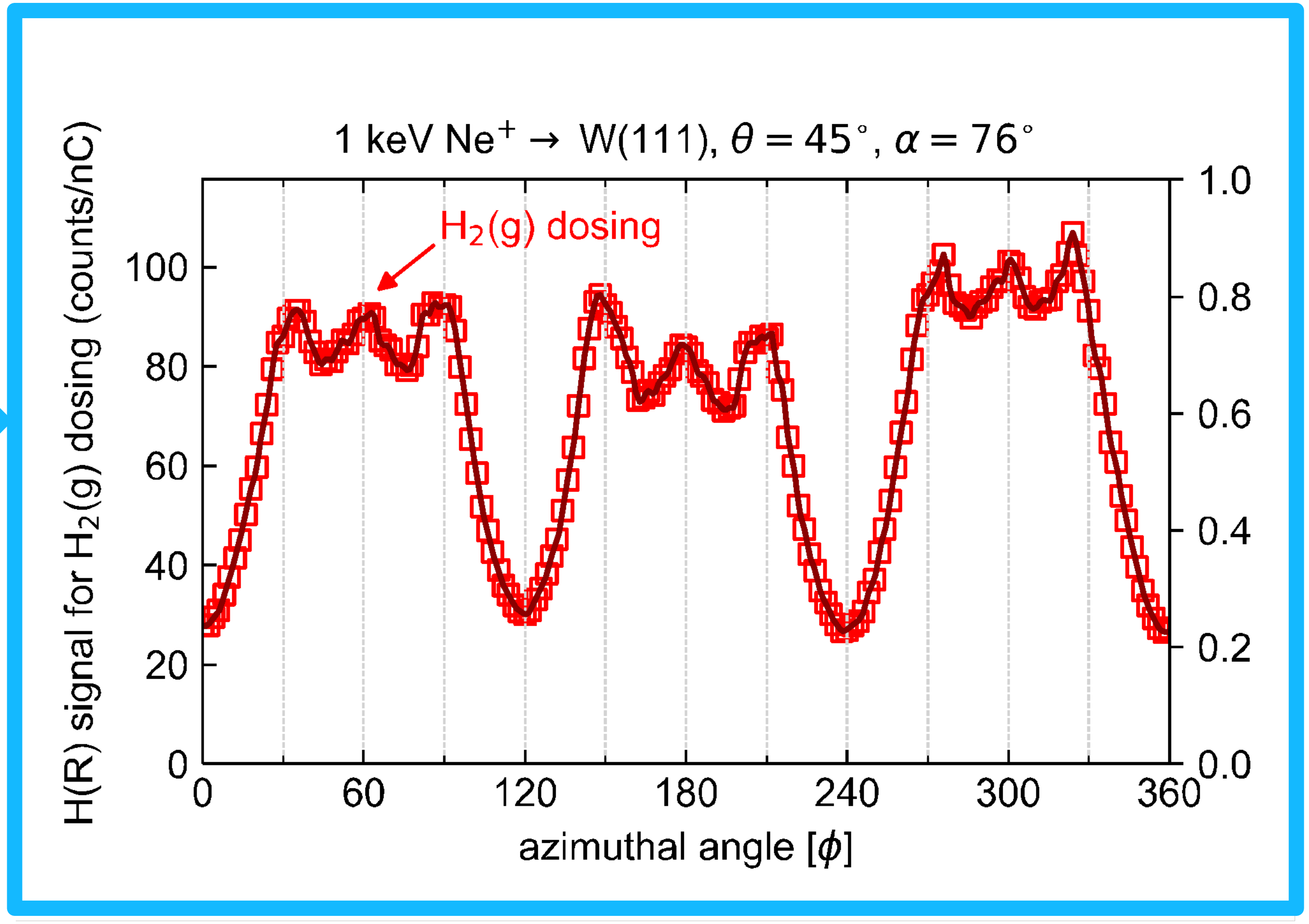
Multi-layer shadow line analysis

- Shadow lines for first 3 layers of W atoms describe map well
- This analysis provides W lattice structure beneath the adsorbed hydrogen



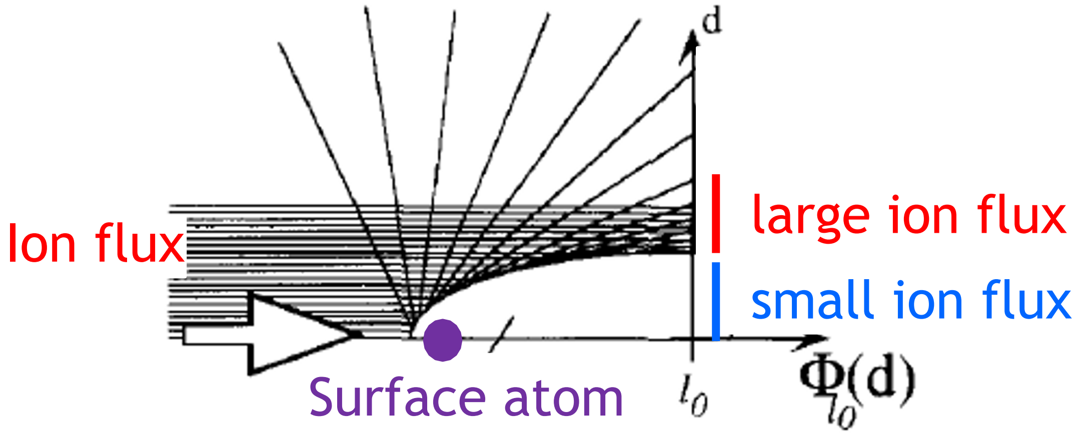
Determining H binding sites





Model this signal to identify H adsorption sites

Shadow cones



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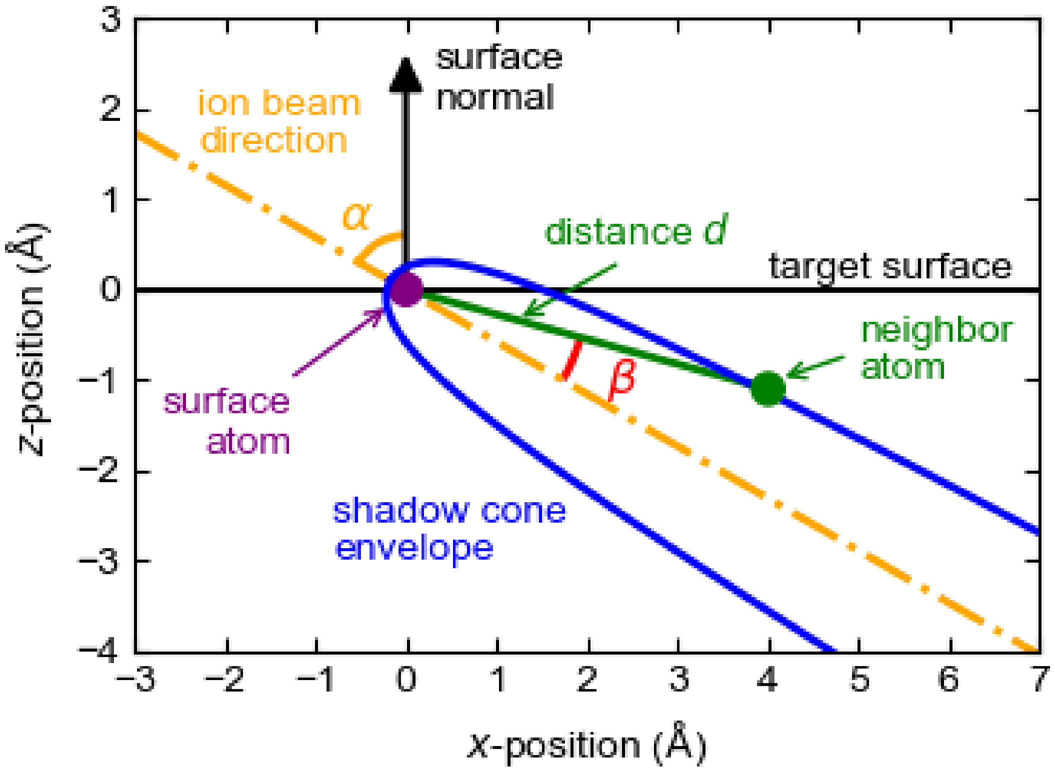

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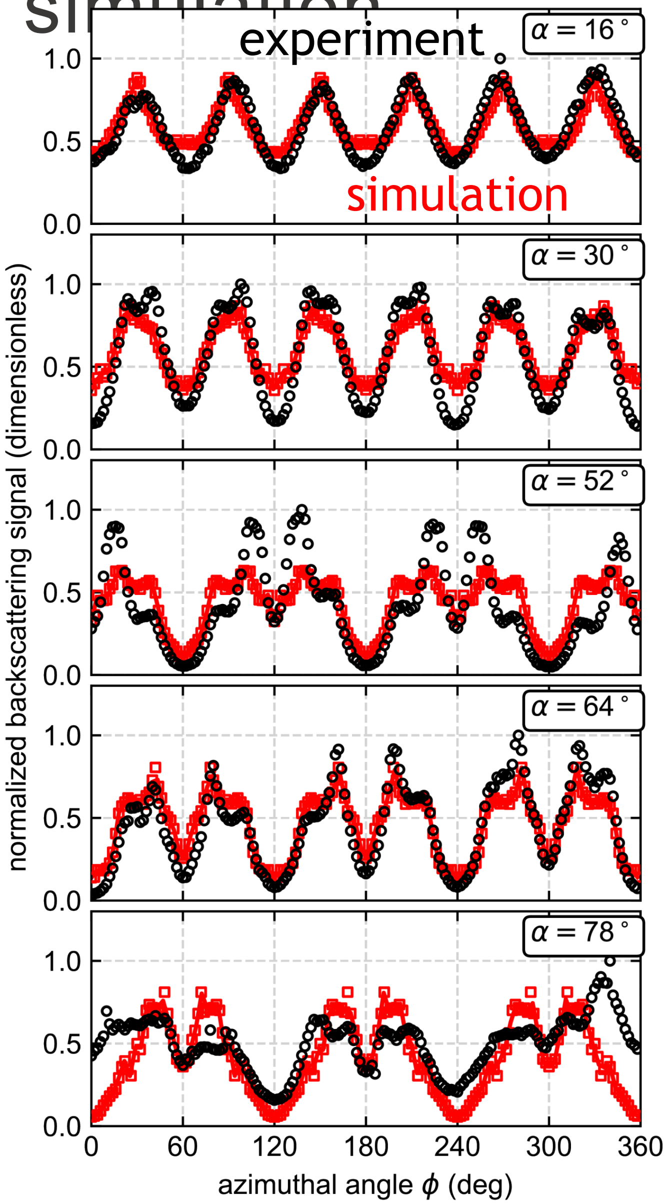
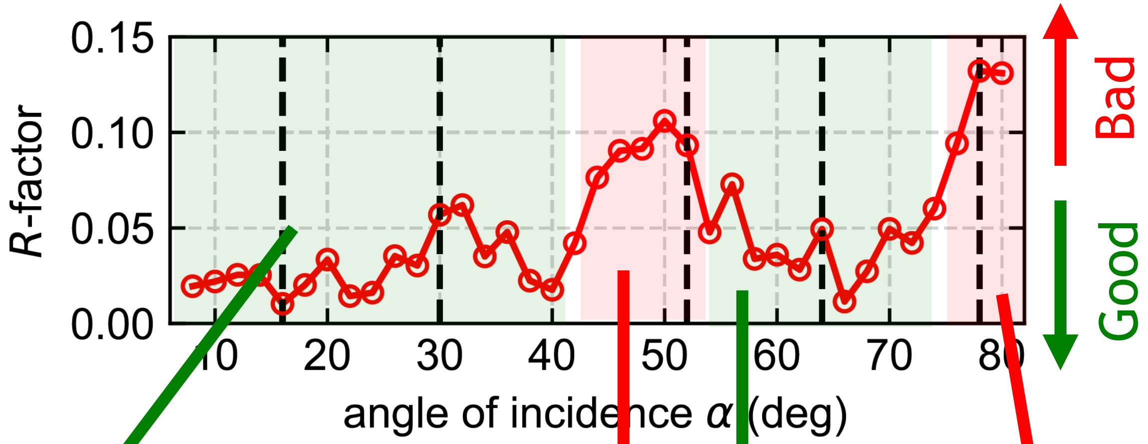
Quantitative comparison between experiment and simulation



R-factor
(least squares fit)



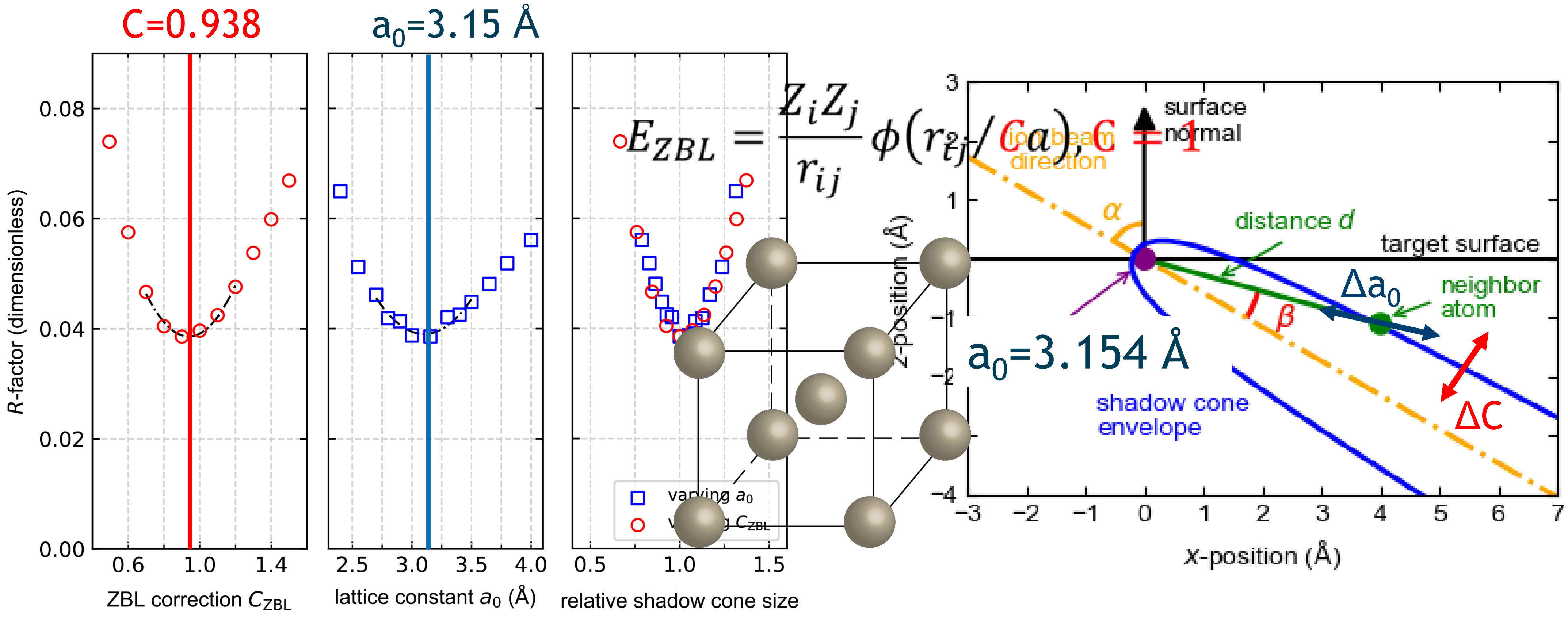
Reasonably good fit, but less sensitive to input parameters since these are for more distant neighbors

Potentially due to experimental imperfections

Glancing angle: BCA breakdown & experimental limits

Reasonably good fit, depends mostly on nearer neighbors

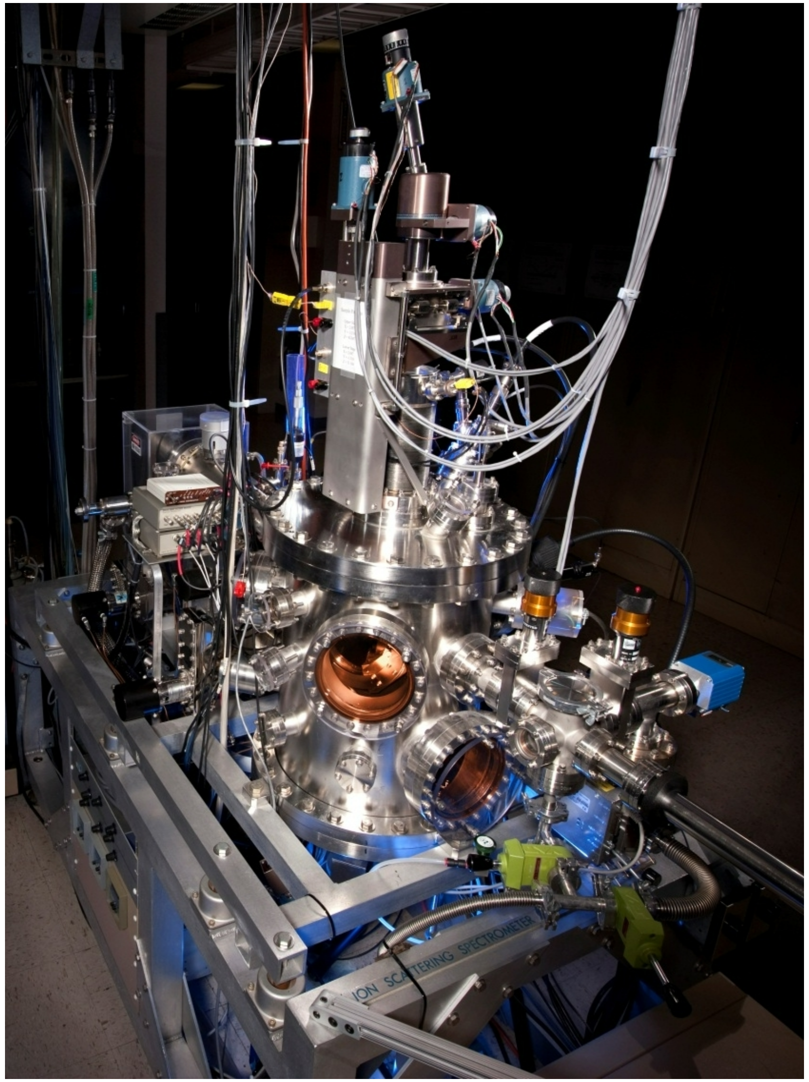
Adjusting inputs in MARLOWE simulation



- ZBL potential does a reasonably good job in describing (3 keV) He-W interaction
- Technique is sufficient to obtain surface structure parameters
- Shadow cone geometry plays a key role in the scattering profile
- Different parameters can affect measurements in the same way (need to be careful!)

Upgraded TOF-ICISS system

Current system: ARIES

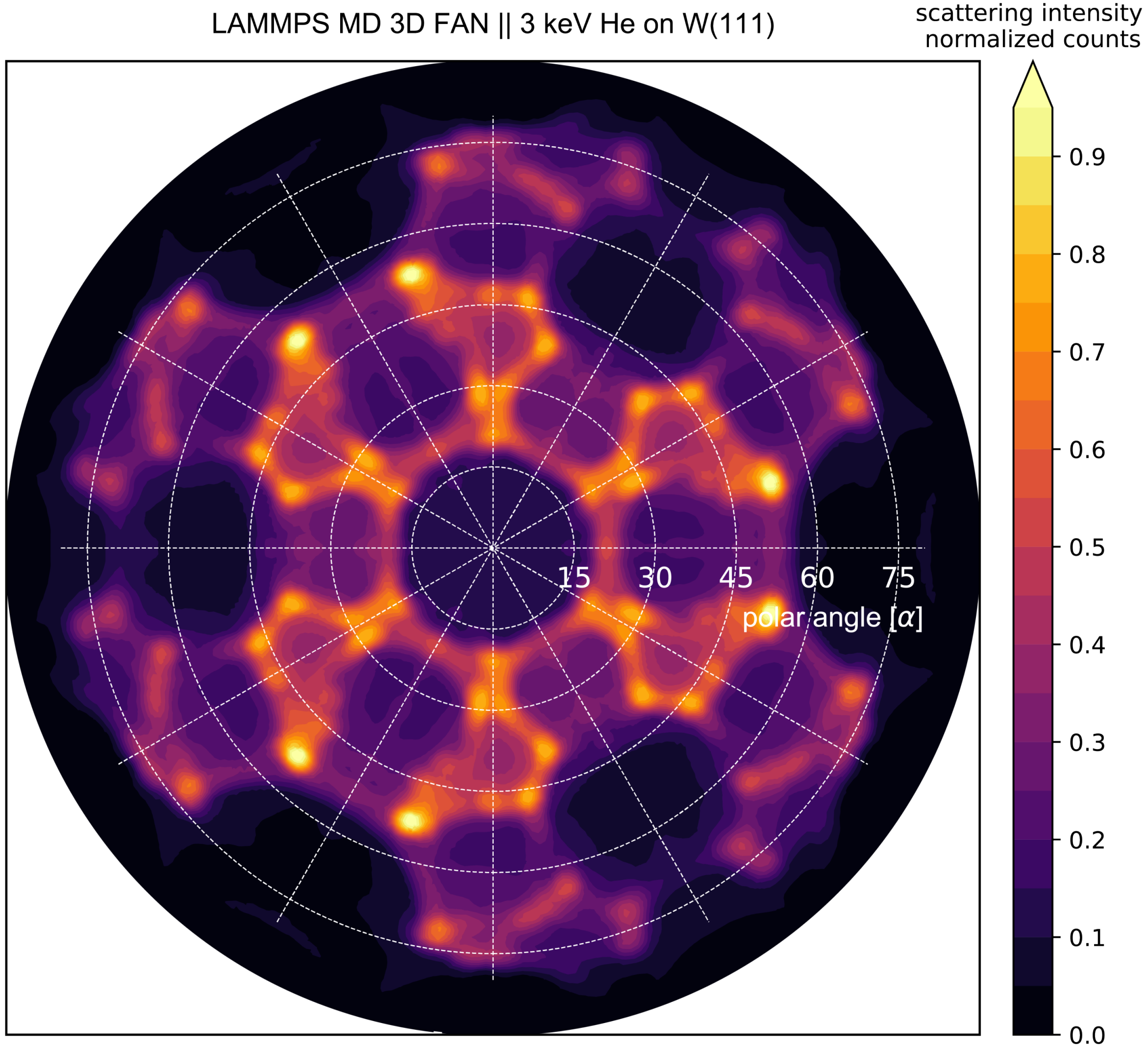


- ARIES is optimized for traditional LEIS (forward scattering), not TOF-ICISS
- An upgraded system designed specifically for TOF-ICISS is currently being assembled at Sandia

- Higher energy ion beam (20 keV Li^+ vs 3 keV He^+)
- Dedicated TOF tubes (>10x longer flight path)
- Smaller detector acceptance angle
- Compatible with plasma source for in-situ exposures
- Real-time measurements during/between exposures

Comparison of current to new system for W(111)

Simulation of current system



Simulation of upgraded system