

Yamashita et al., Scientific Reports 8:12325 (2018)

Examples of quantitative STEM

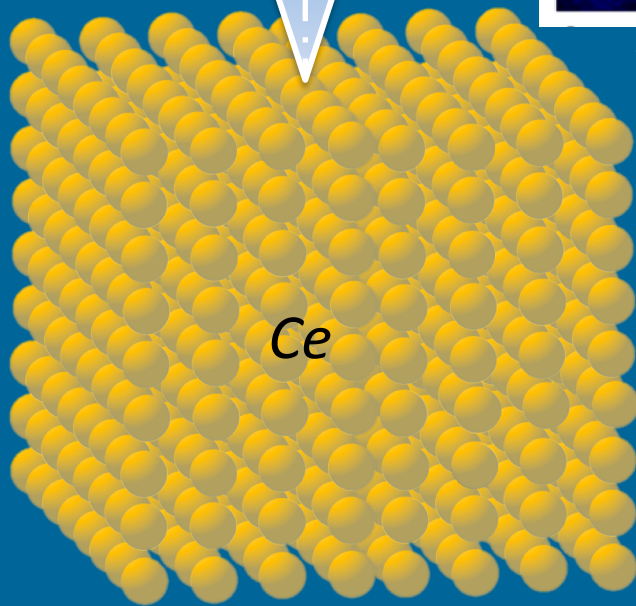
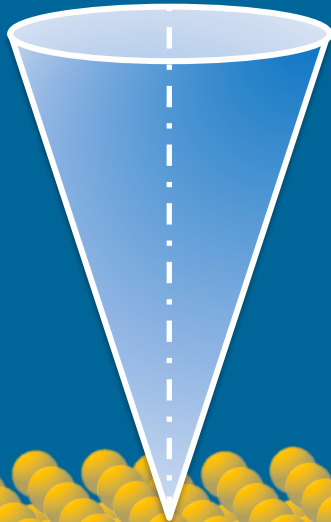
First Example

3D position of a single Ce dopant atom in an AlN crystal

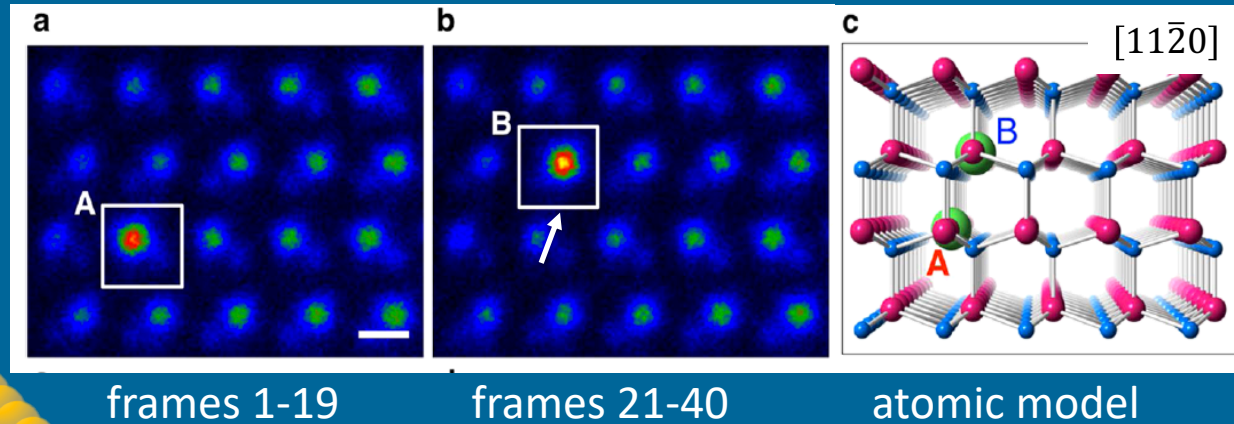
R. Ishikawa et al. NanoLetters 14, 1903 (2014)

3D position of a single Ce dopant atom in an *w*-AlN crystal

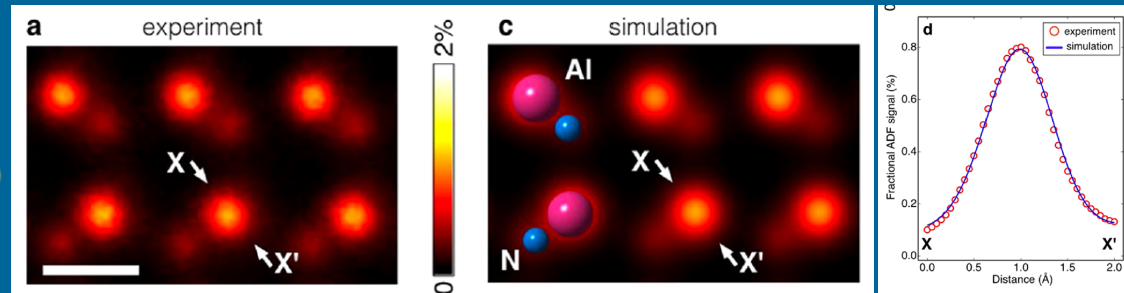
R. Ishikawa et al. NanoLetters 14, 1903 (2014)



took 40 frames to reduce noise



Step 1:

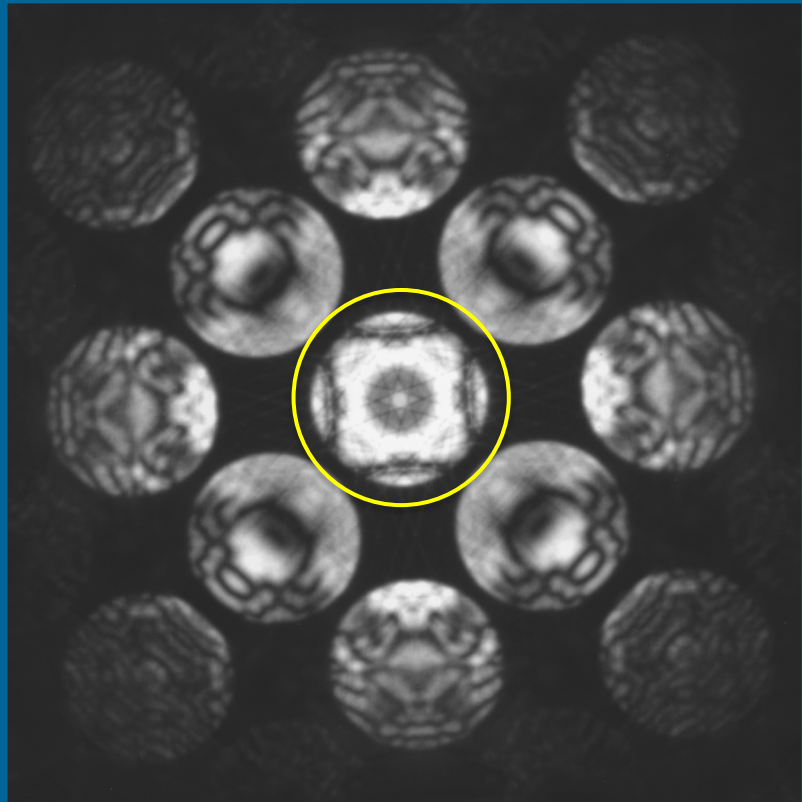
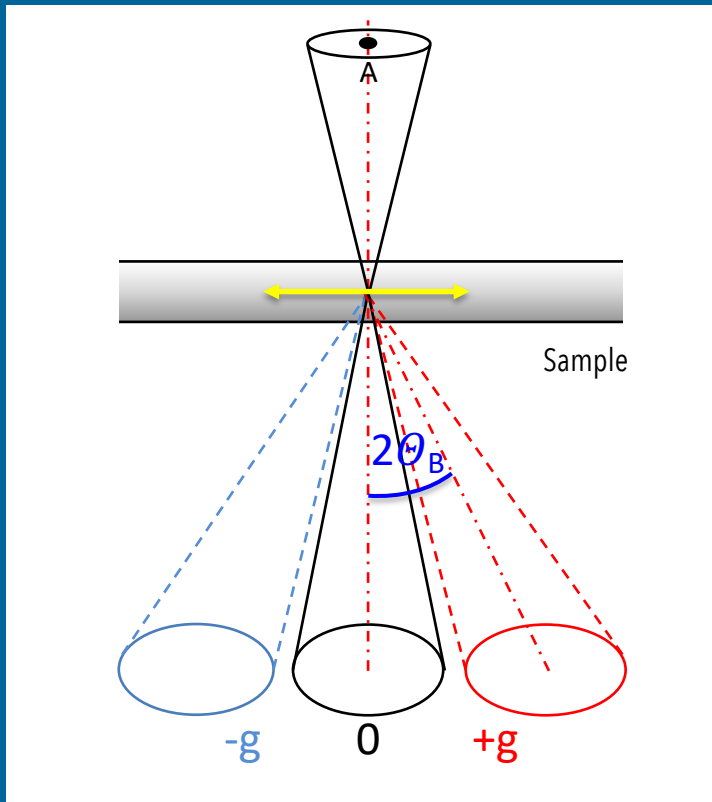


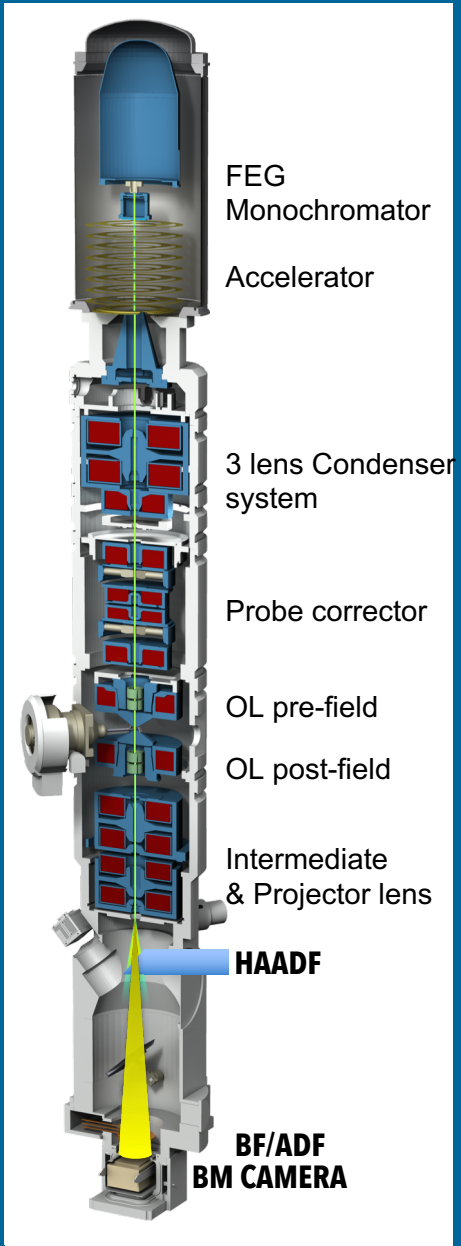
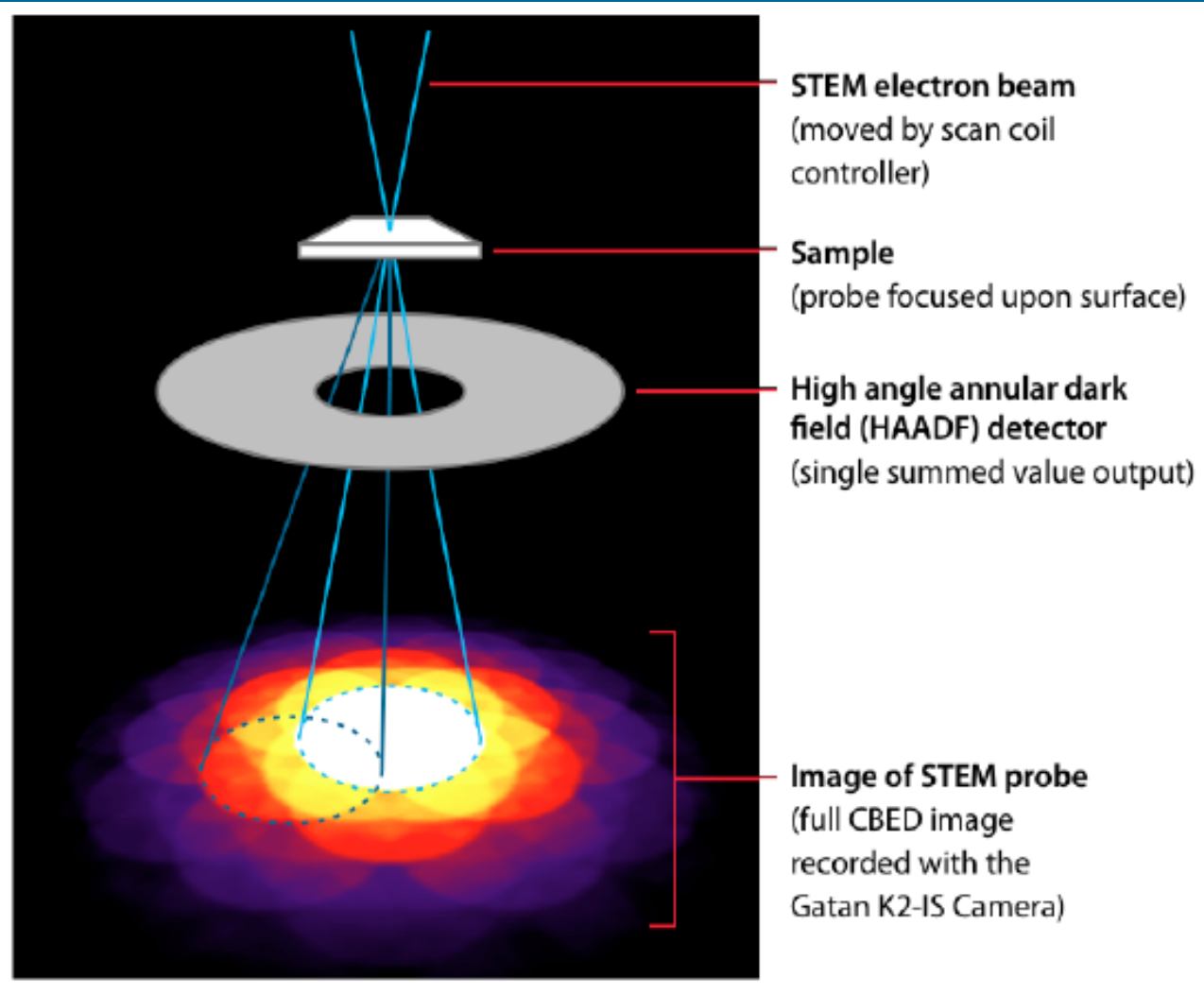
establish probe shape by image simulation

Step 2: Determine thickness

Position averaged convergent beam electron diffraction (PA-CBED)

J. LeBeau et al., Ultramicroscopy 110, 118 (2010)



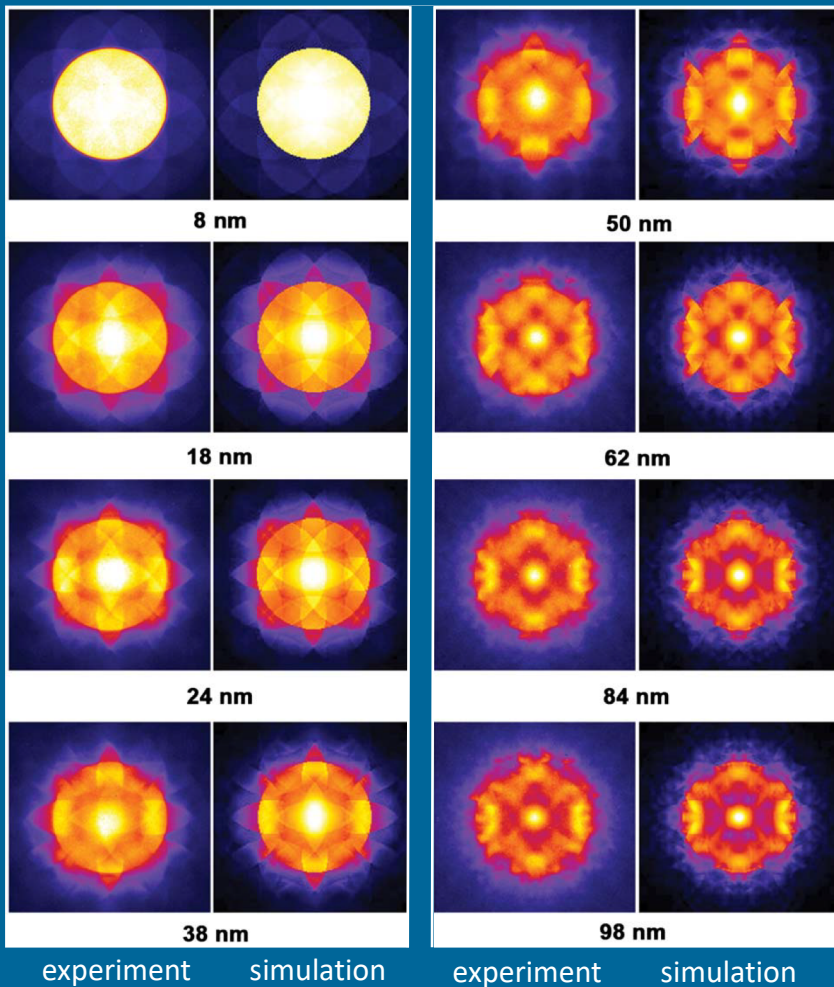


C. Ophus et al., M&M 2014
4 D STEM

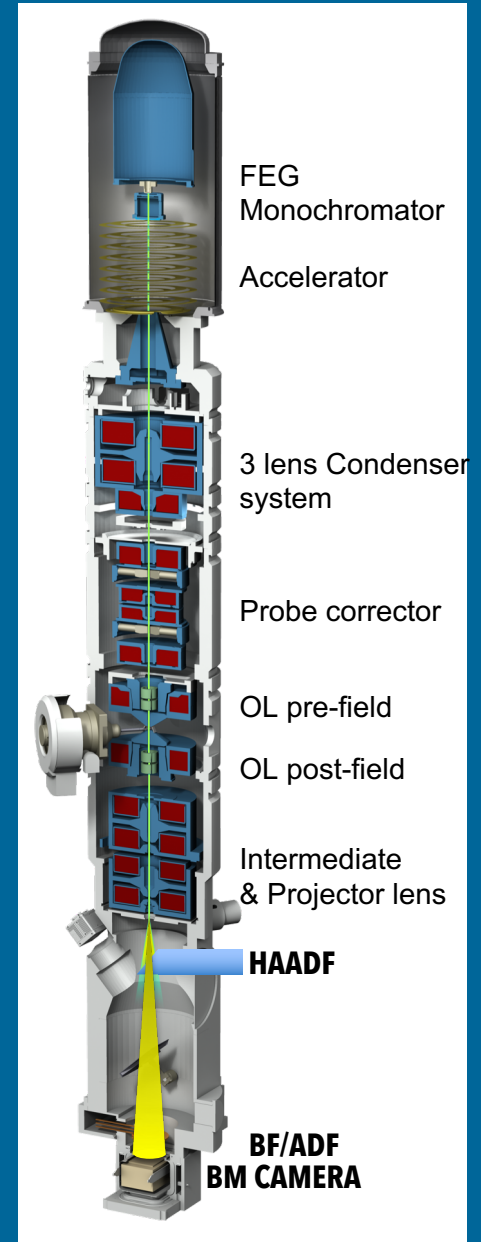
Position averaged convergent beam electron diffraction (PA-CBED)

J. LeBeau et al., Ultramicroscopy 110, 118 (2010)

$\alpha = 9.5 \text{ mrad}$, 300 keV



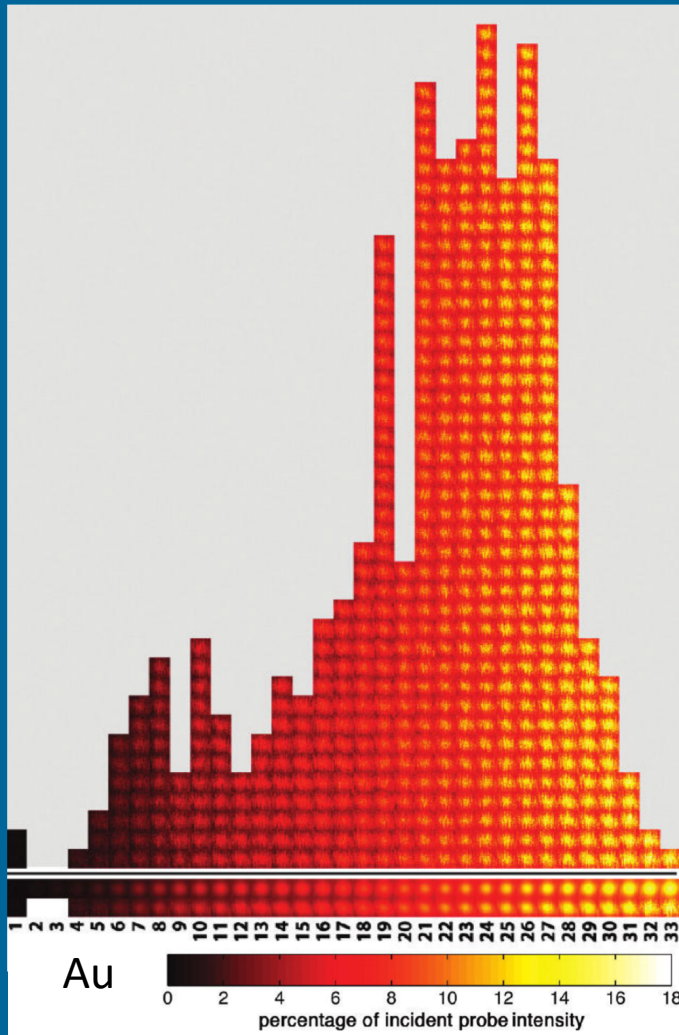
PA-CBED patterns:
experimental /simulated yield
specimen thickness **to < 10%**



Atom counting

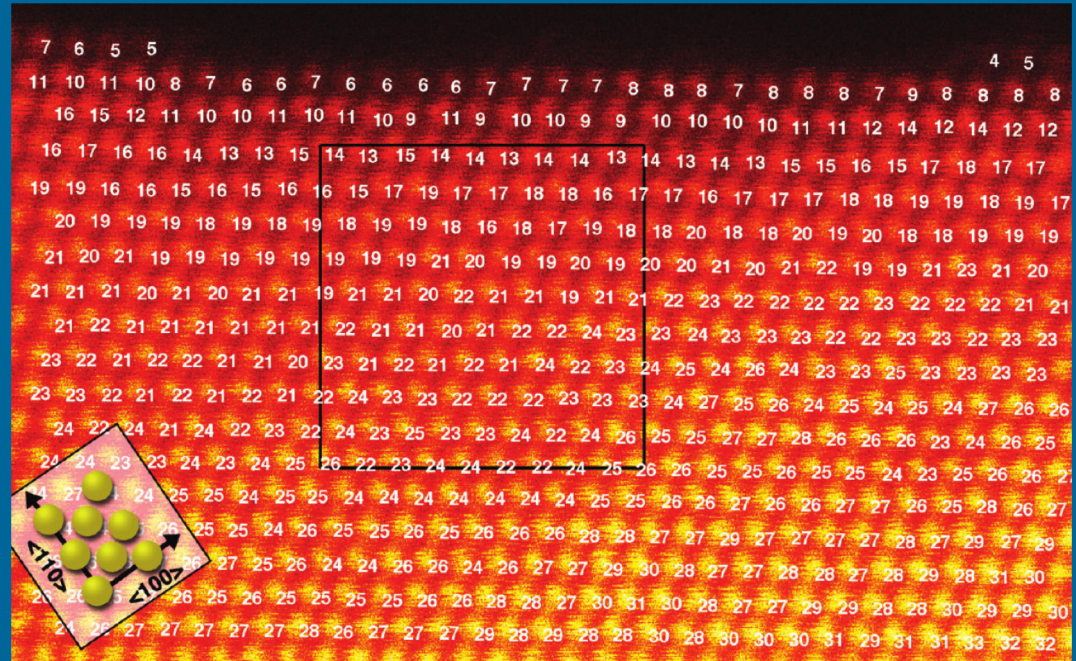
J. LeBeau et al., NanoLetters 10, 4405 (2010)

example of gold



Number of atoms in column

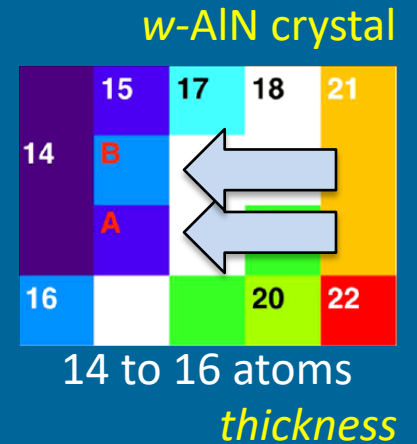
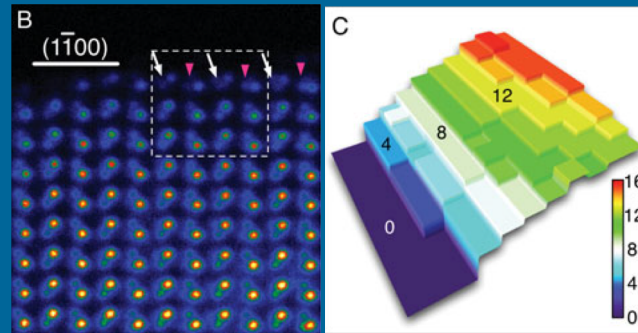
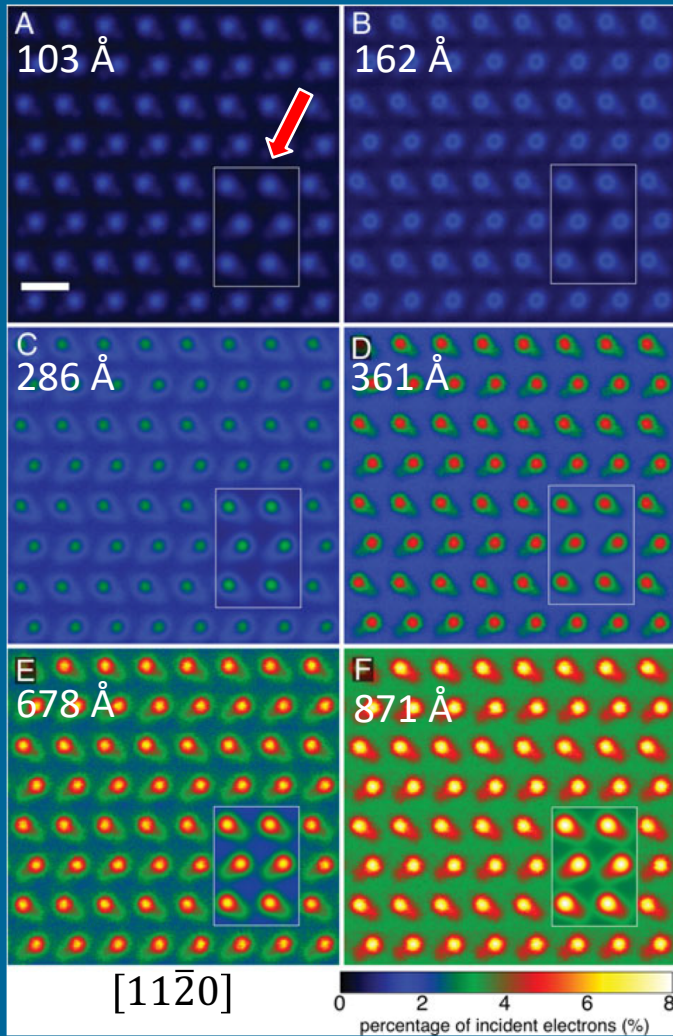
Au [110]



Measurement of intensities on absolute scale
& matching by image simulations
yields number of atoms per column

Atom counting by absolute intensity measurements

R. Ishikawa et al. NanoLetters 14, 1903 (2014)



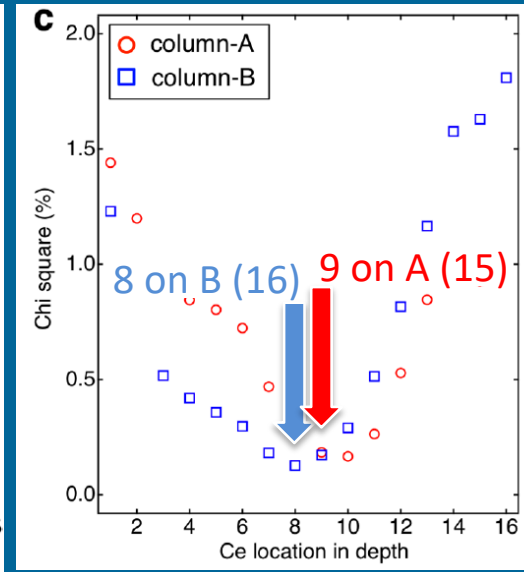
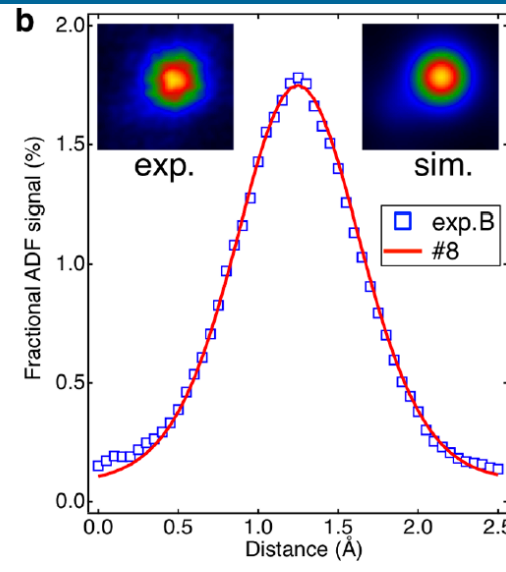
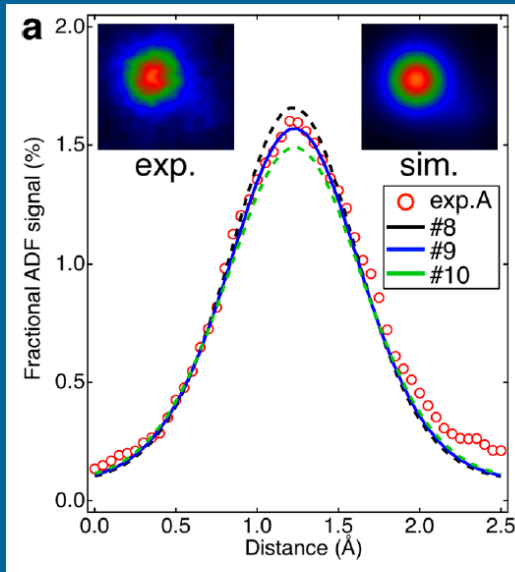
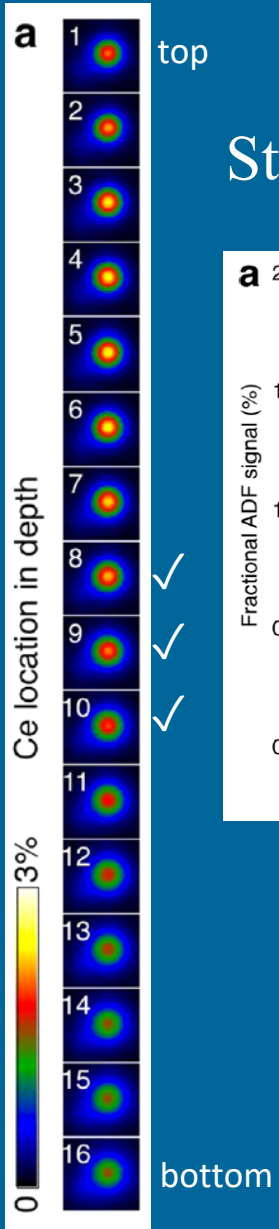
establish sample thickness by atom counting
on basis of absolute intensity measurements

R. Ishikawa et al., Microsc- Microanal. 20, 99 (2014)

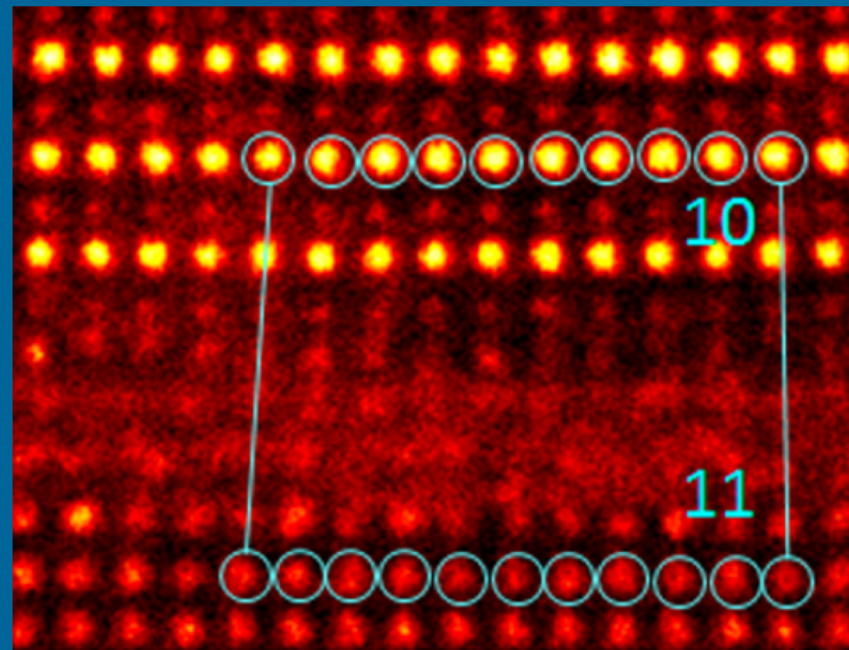
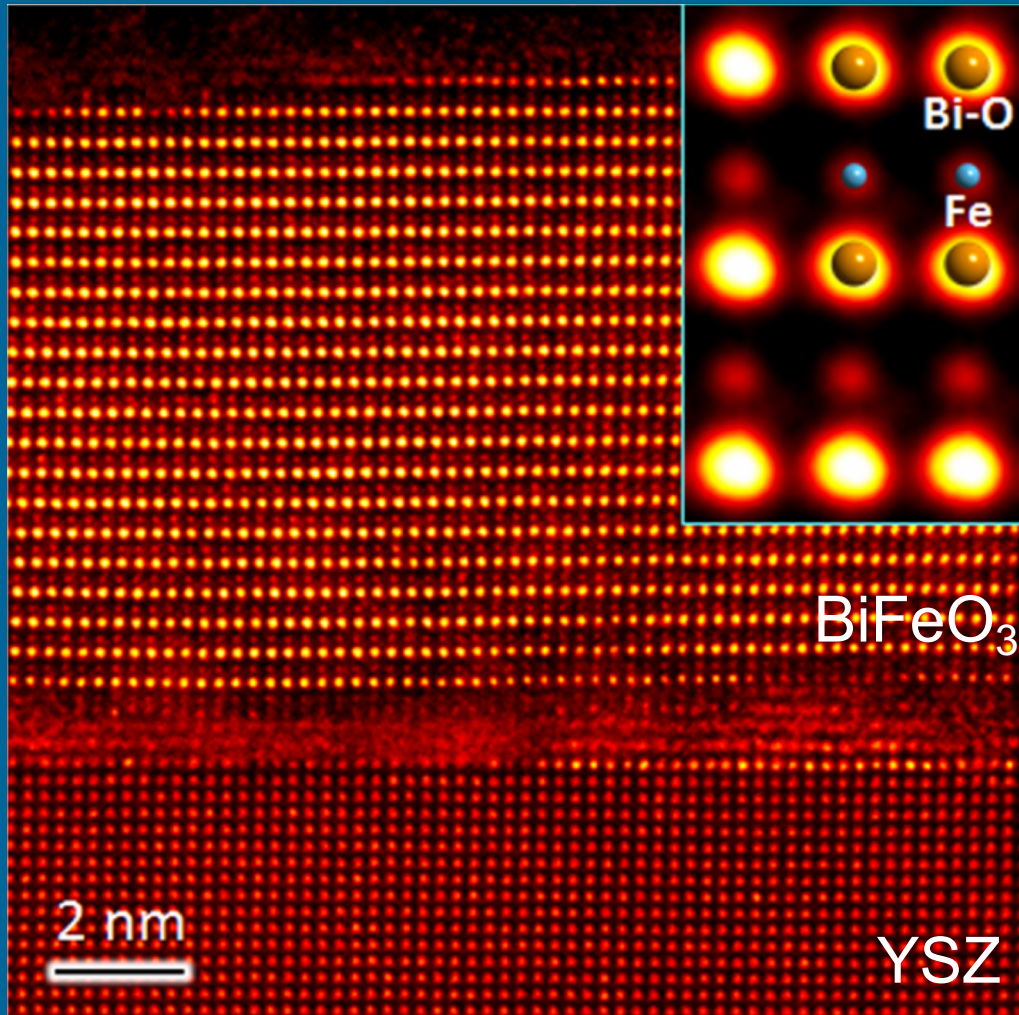
3D position of a single Ce dopant atom in an *w*-AlN crystal

R. Ishikawa et al. NanoLetters 14, 1903 (2014)

Step 3: Where (in depth) is the atom?



BiFeO₃ on yttria-stabilized zirconia



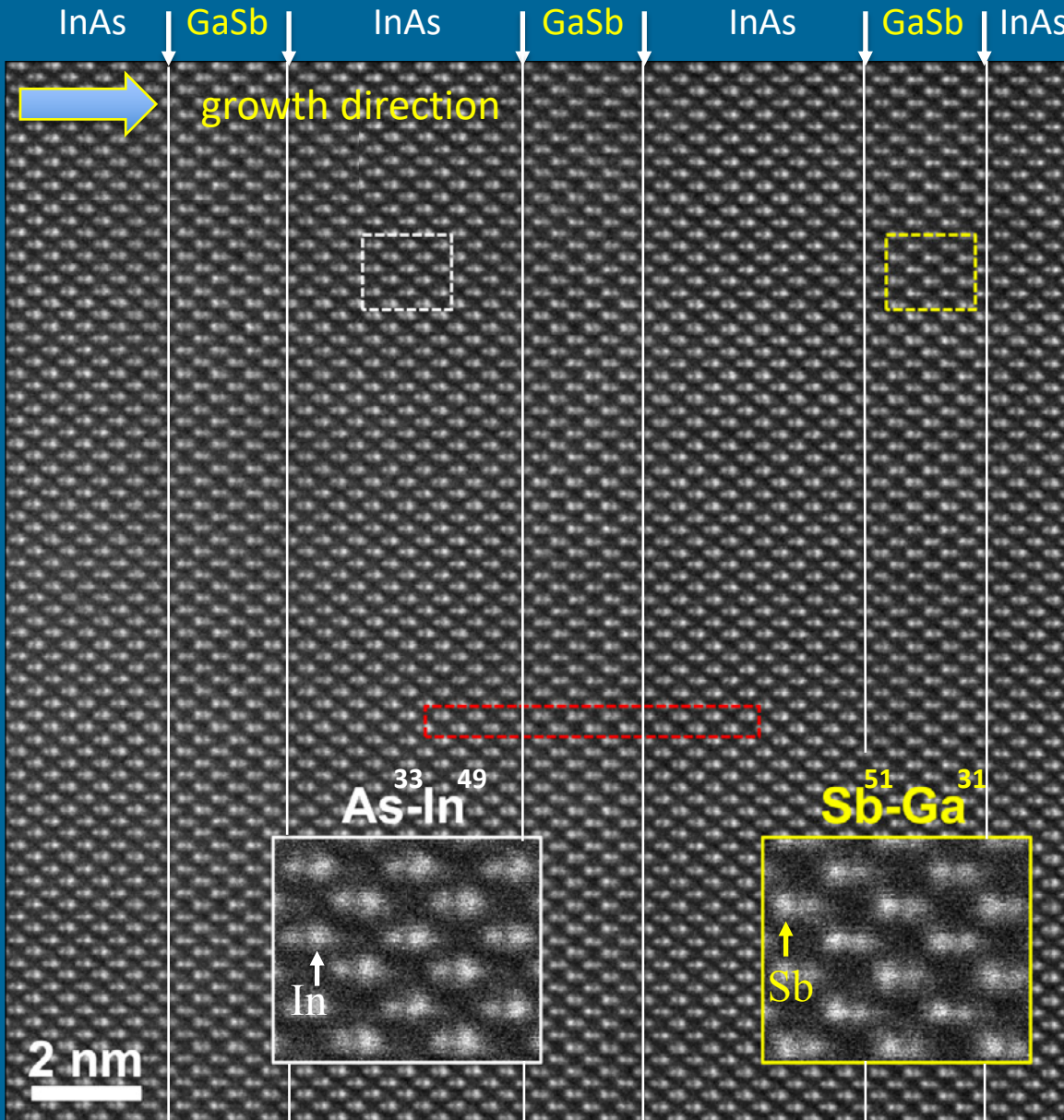
Bi⁸³ Fe²⁶ Zr⁴⁰ O⁸

Examples of quantitative STEM

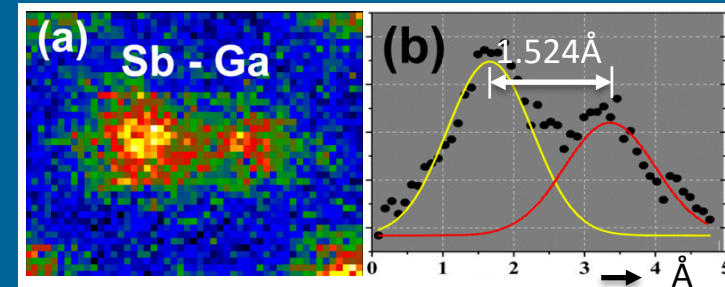
Second Example

Picometer precision measurement of strain at InAs/GaSb interface

H. Kim, J.-M. Zuo, *Micron* 92, 6 (2017)



- 300 keV
- probe: 23.5 mrad (size 0.7 Å)
- HAADF detector: 60 to 370 mrad

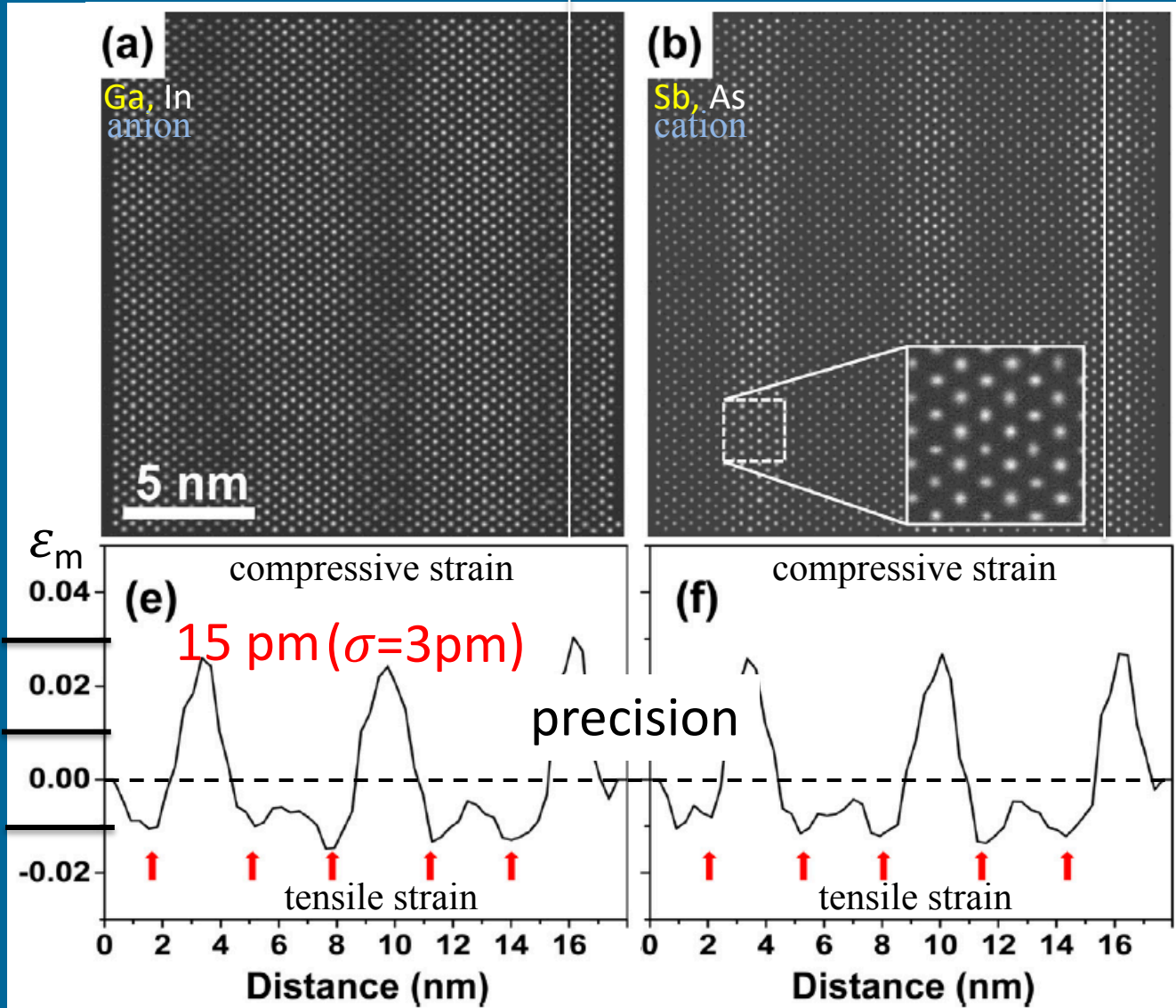


- quantitative image simulation
- construct separate Ga/In and Sb/As sublattice
- measure with respect to ideal sublattice

Picometer precision measurement of strain at InAs/GaSb interface

H. Kim, J.-M. Zuo, *Micron* 92, 6 (2017)

GaSb InAs GaSb InAs GaSb GaSb InAs GaSb InAs GaSb



$$\epsilon_m = \frac{a - d_{\text{GaSb}}}{d_{\text{GaSb}}}$$

+18 pm
+6 pm
0
-6 pm

precision

15 pm ($\sigma=3\text{pm}$)

tensile strain

compressive strain

(f)

tensile strain

Distance (nm)

Distance (nm)

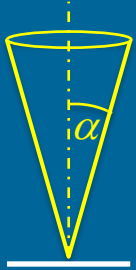
Annular Bright Field (ABF)

STEM: Atomic resolution imaging easily accessible

Pay attention to
Quantitative details of ADF/HAADF imaging in STEM

SiC [011] at 300 keV

(N. Lugg, Thesis Univ. Melbourne 2011)



$\alpha = 8.5$ mrad

$\alpha = 12.5$ mrad

$\alpha = 16.5$ mrad

$\alpha = 20.2$ mrad

C⁶

C

C

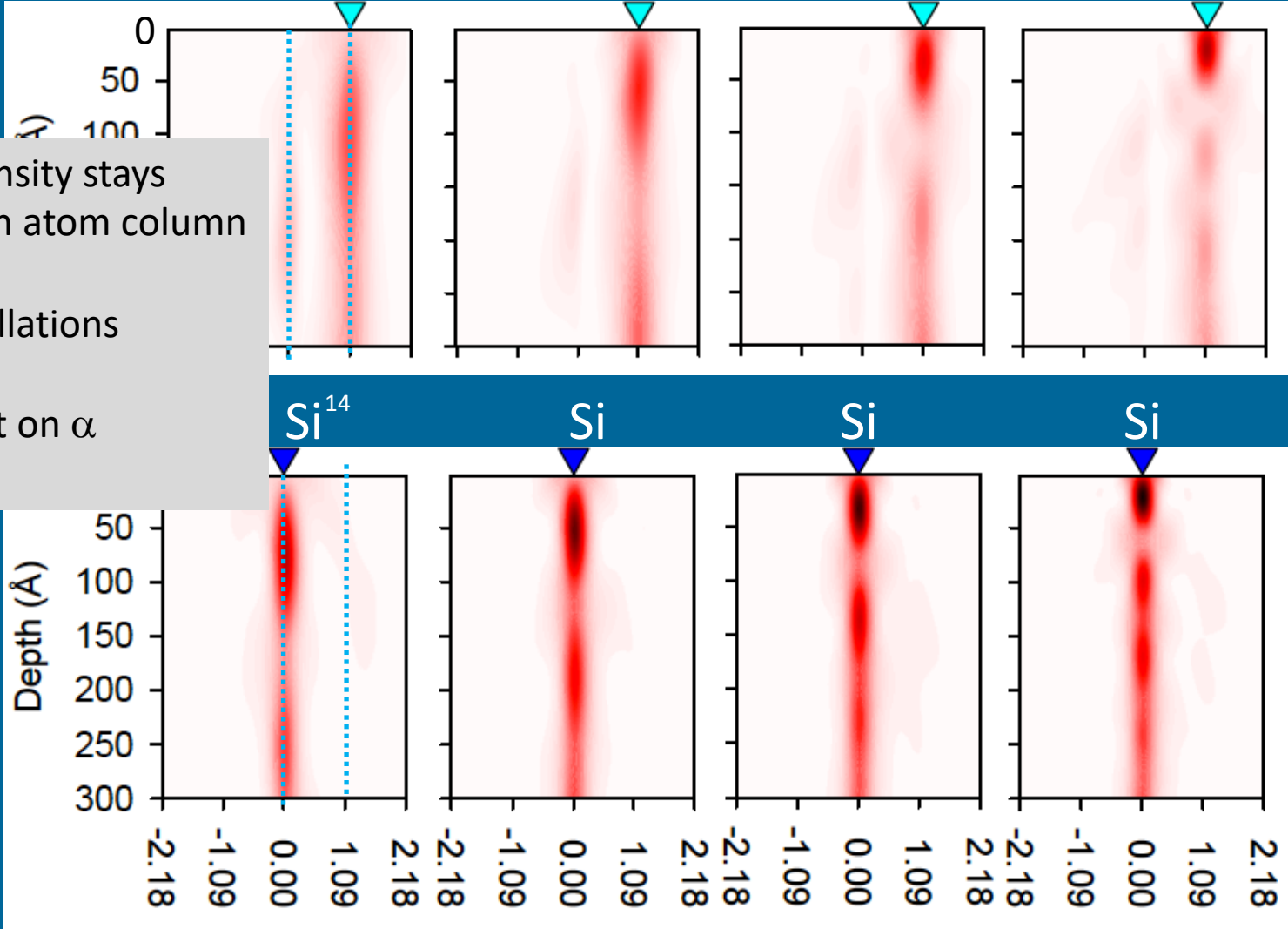
C

Si¹⁴

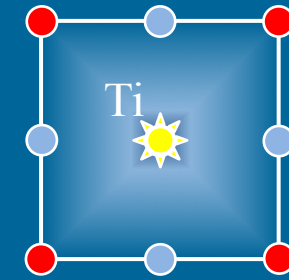
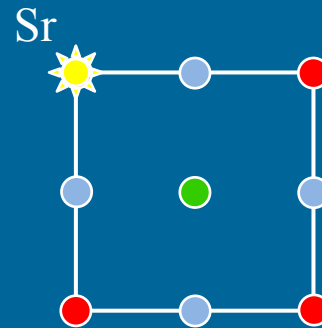
Si

Si

Si

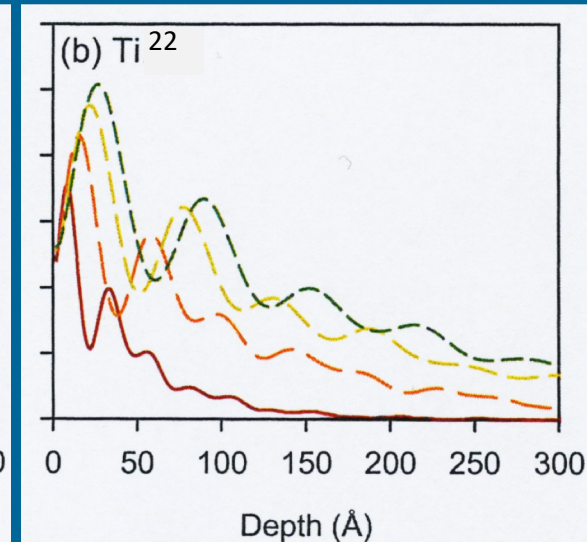
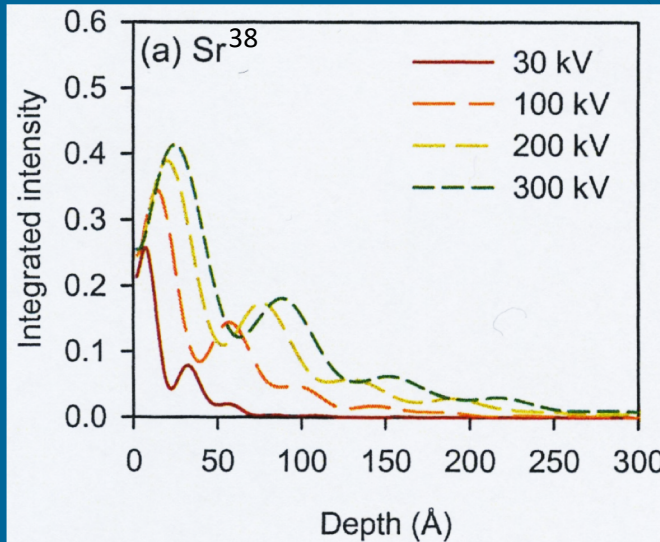


- Probe intensity stays localized on atom column
- Depth oscillations
- Dependent on α



$\alpha = 17 \text{ mrad}$

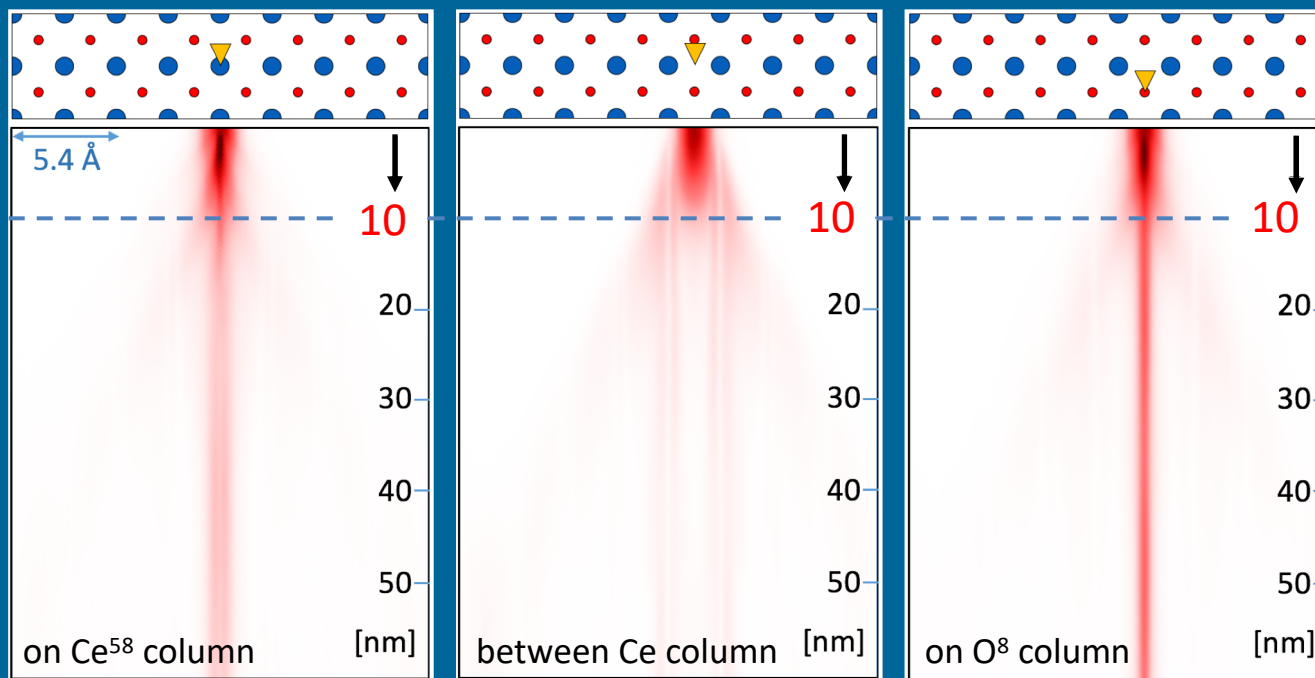
- Probe intensity stays localized on atom column
- Depth oscillations
- Dependent on α
- Intensity on atom column decreases with depth
- Dependent on e-energy
- Dependent on Z



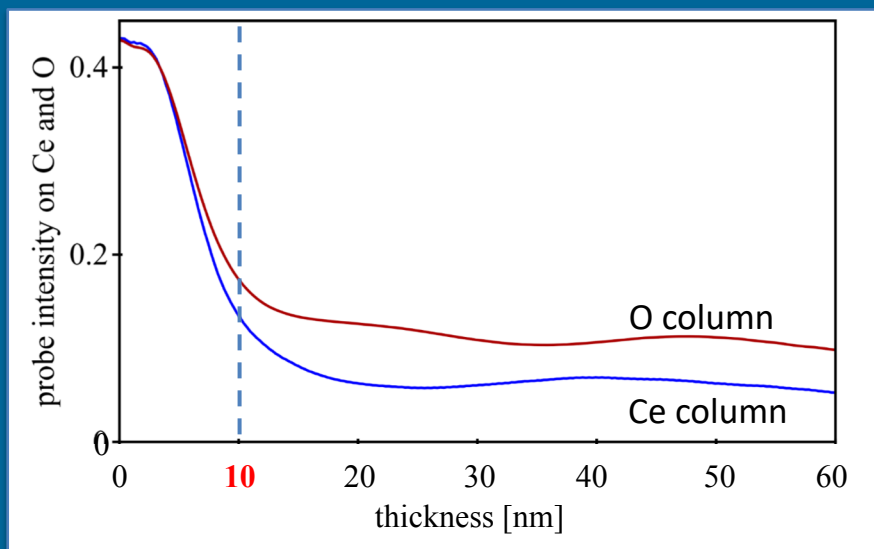
Redistribution of e-intensity:

- the atom columns are origin of inelastic scattering
- intensity is scattered in between the columns

CeO₂ [001] (J. Barthel) Thick samples ?



$\alpha=20$ mrad
1 Å probe
300 keV

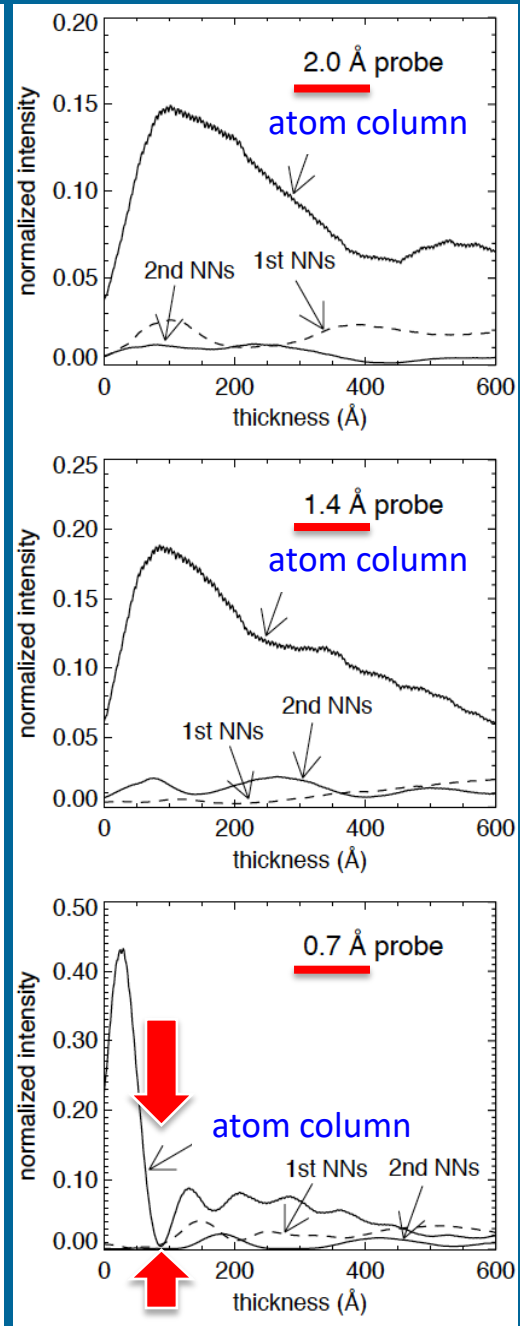
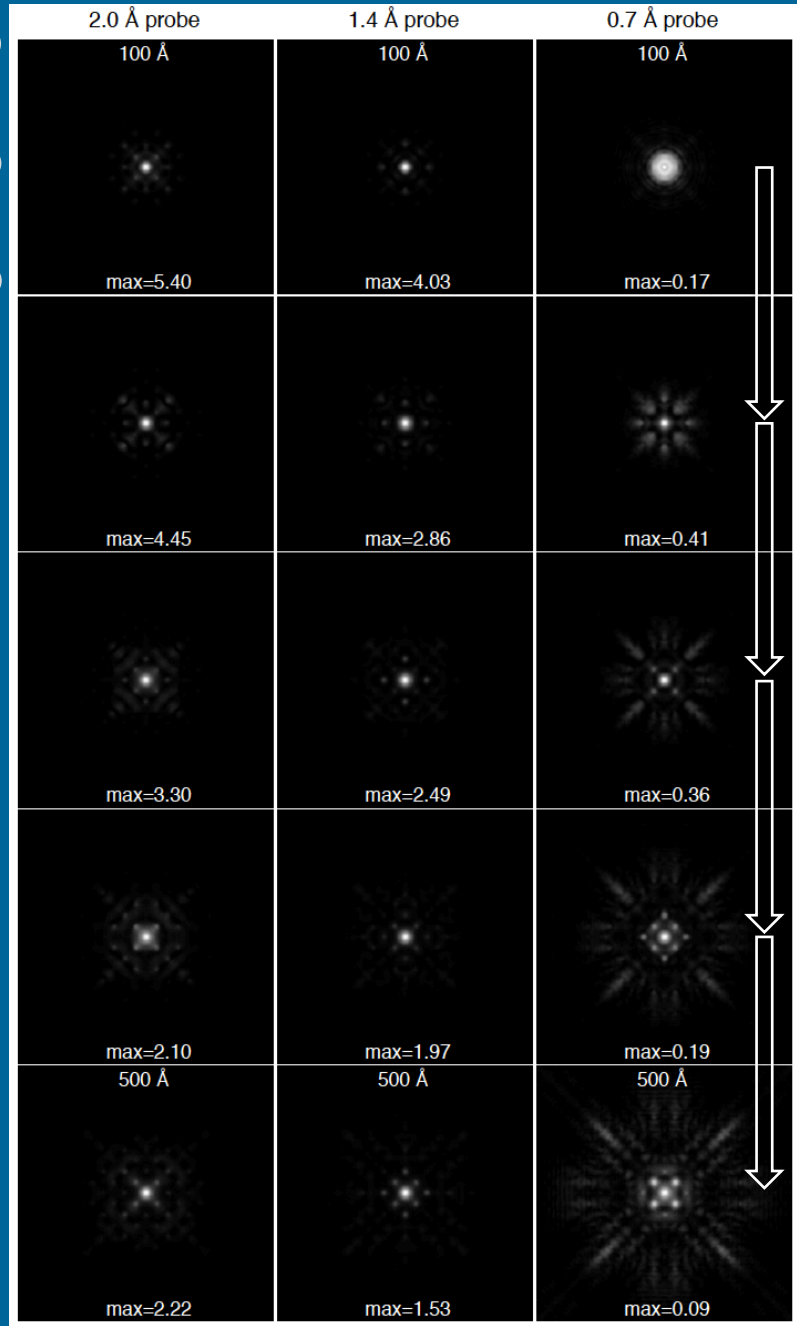
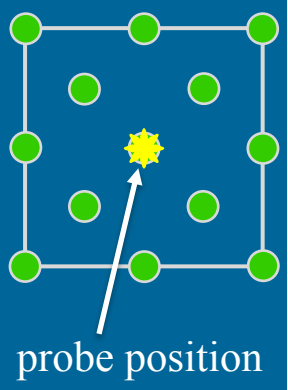


Thick samples ?

- Yes
- However:
information mainly from 10 nm surface area

Si [001]

(C. Dwyer, J. Etheridge, Ultramicroscopy 96, 343 (2003))



(10 mrad)



larger beam
less convergence
less transverse momentum

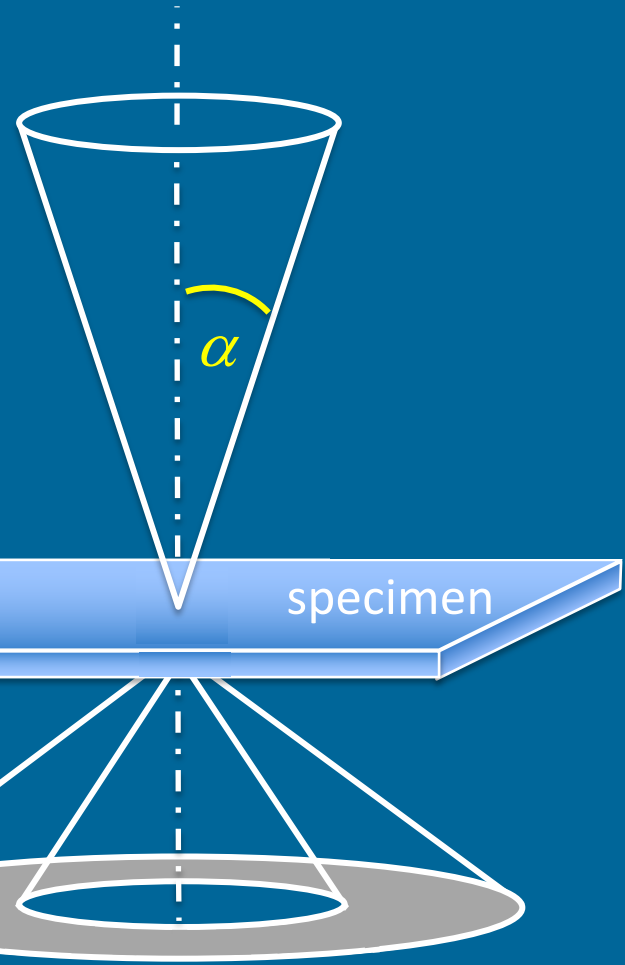
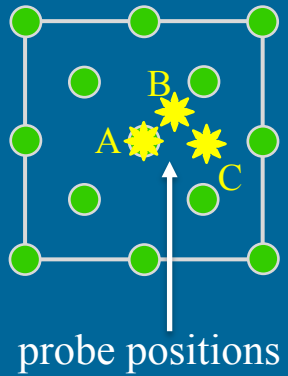
(30 mrad)



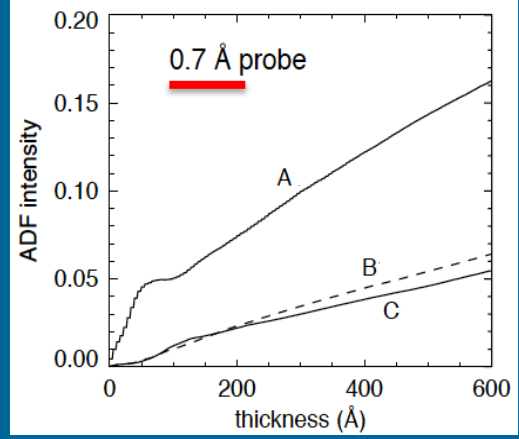
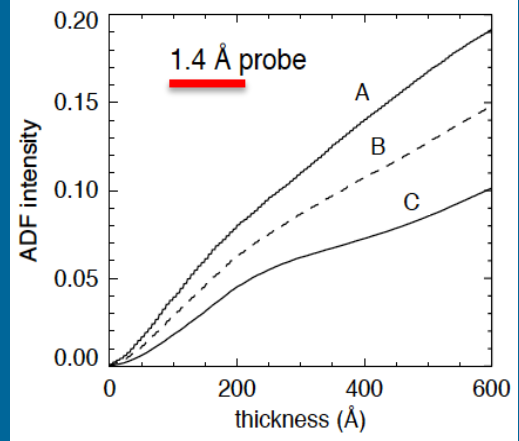
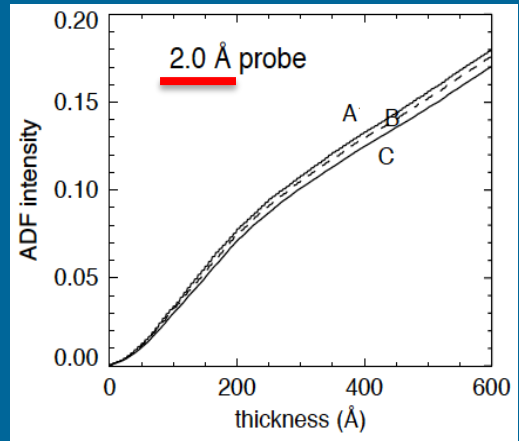
small beam
high convergence
high transverse momentum

Si [001]

(C. Dwyer, J. Etheridge, Ultramicroscopy 96, 343 (2003))



(HA)ADF (50 – 150 mrad)

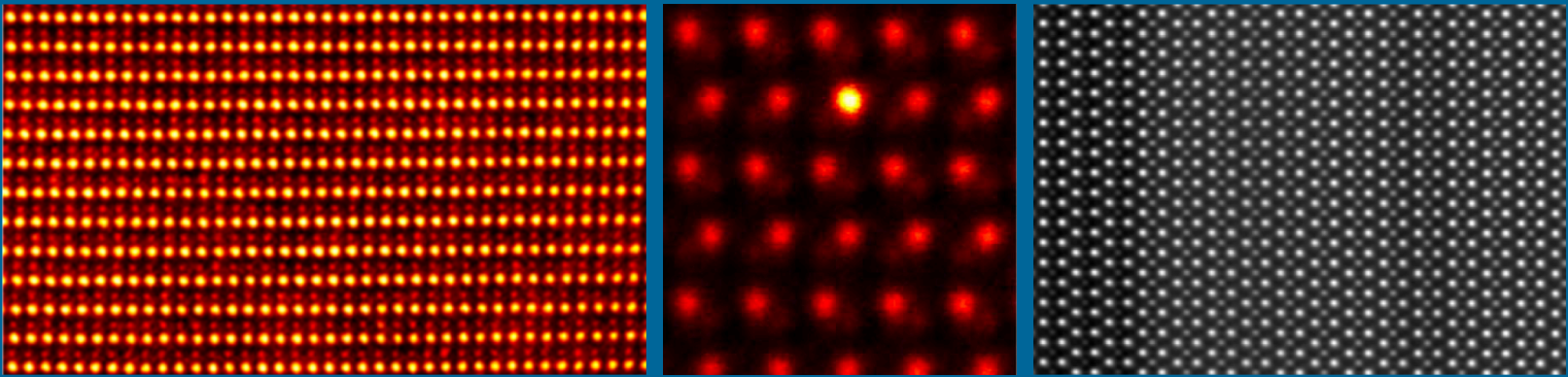


(10 mrad)



(30 mrad)





STEM: Atomic resolution imaging easily accessible

Quantitative aspects of ADF/HAADF imaging in STEM

- Signal to noise; $Z^{2-\delta}$
- Depth oscillations on atom columns (not on ADF total signal)
- Dependent on probe conv. angle α
- Intensity on atom column decreases with depth
- Dependent on e-energy
- Integrated (HA)ADF signal depends on probe conv. angle α
- Depends on thickness
- Sample tilt
- Beam: Lens aberrations
- Detector „illumination“

➔ Measurement of imaging parameters

➔ Image calculations compulsory