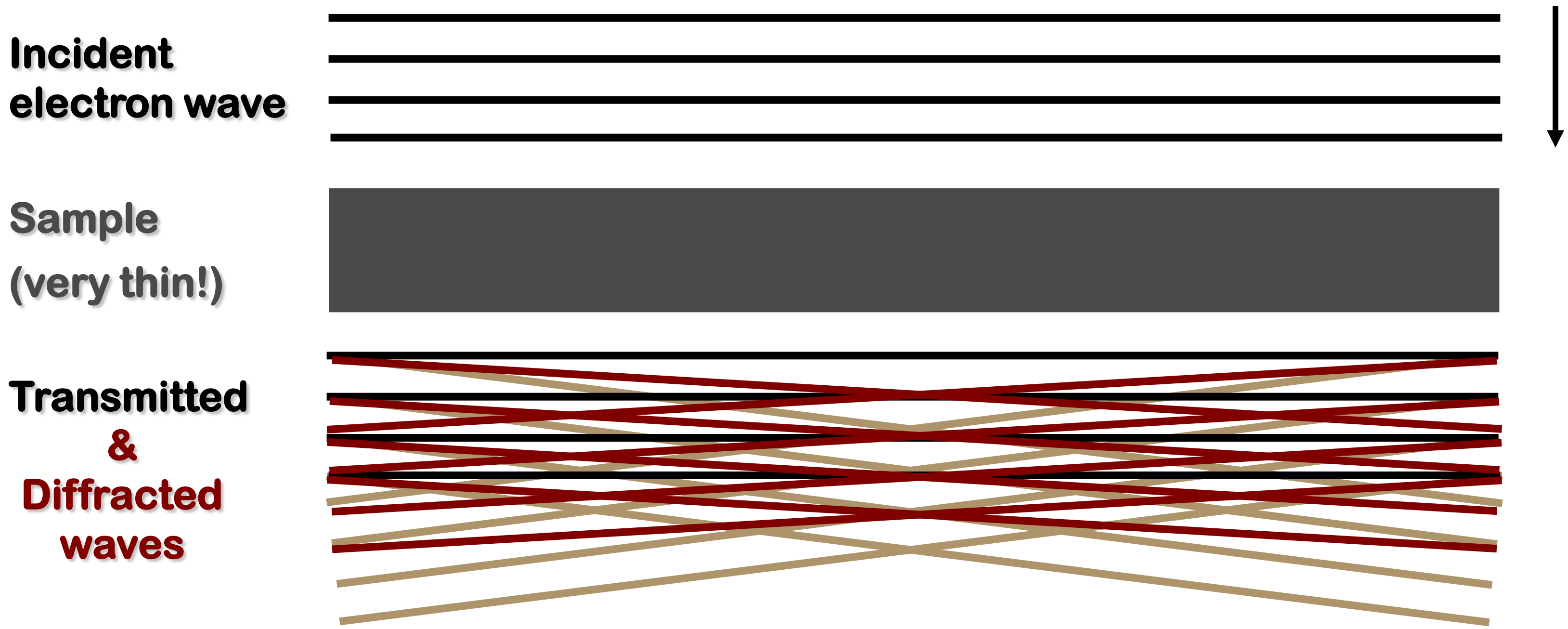
Overview of High-Resolution TEM & Scanning TEM

Lecture 11

High-resolution EM

general idea



Transmitted & diffracted waves each have a different phase

Result is an interference pattern - our ‘phase contrast’ or HREM image

High-resolution EM
general idea

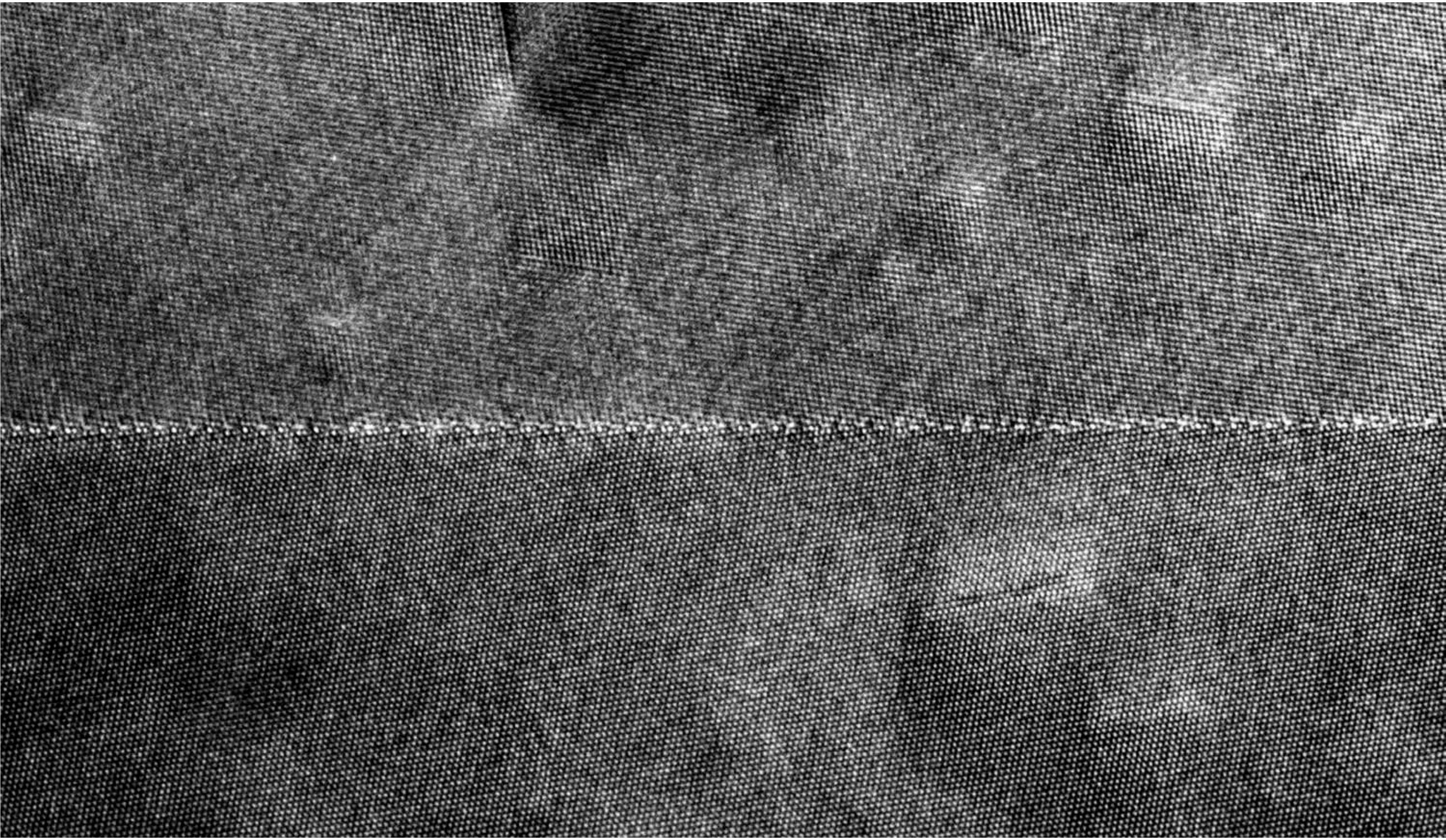


Image courtesy U. Dahmen, NCEM, LBNL

High-resolution EM
general idea

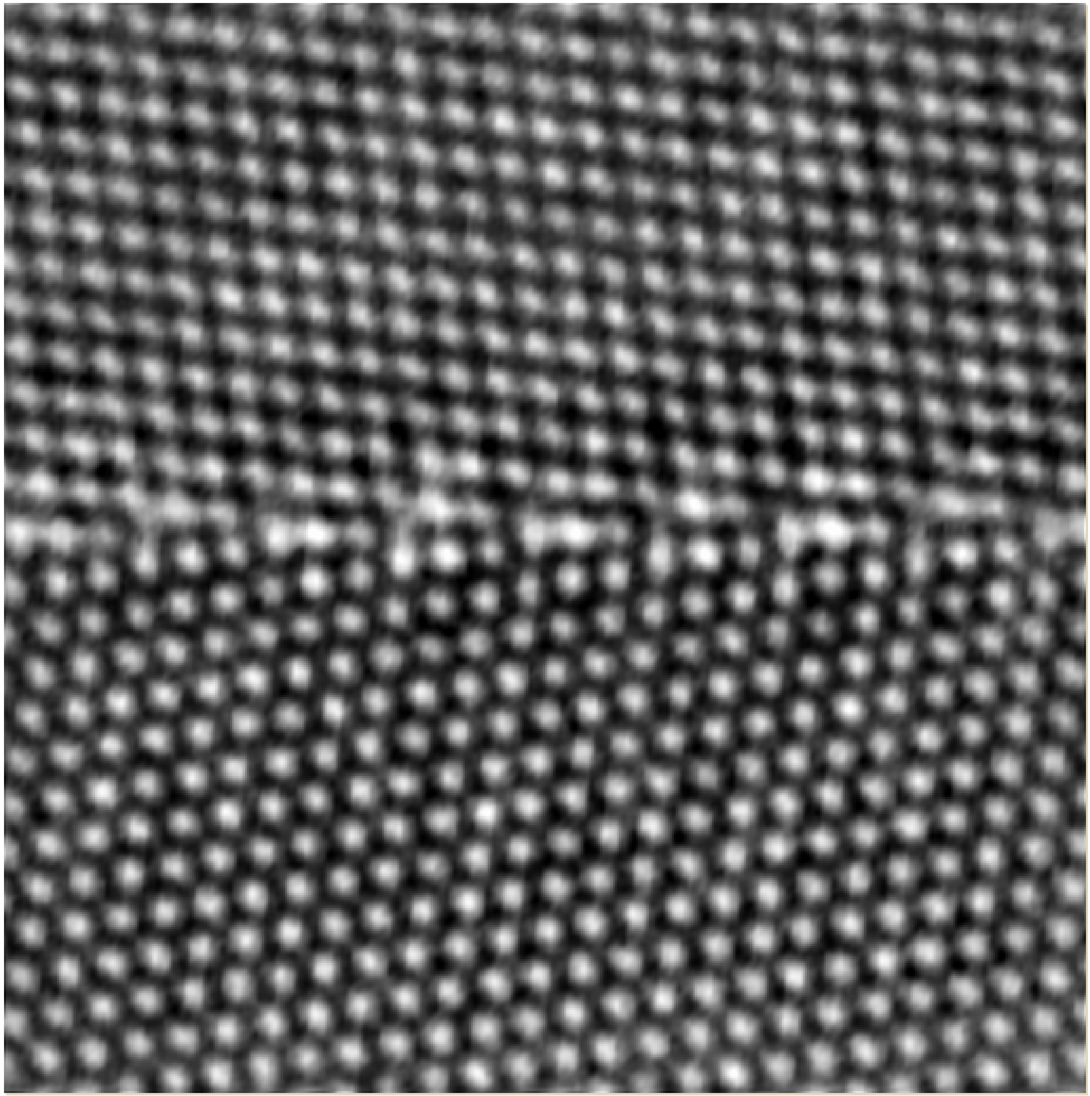


Image courtesy U. Dahmen, NCEM, LBNL

High-resolution EM
general idea

Why are the phases different?

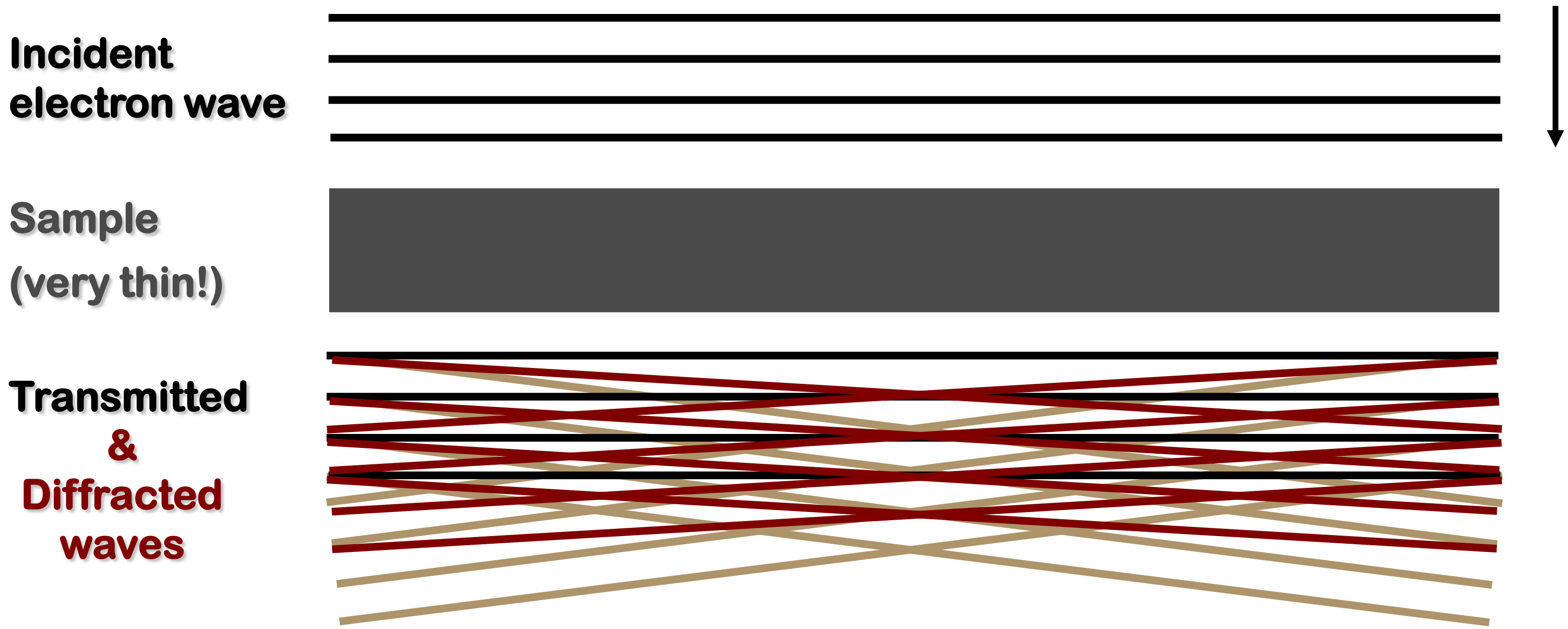
Transmitted & diffracted waves travel different distances in the crystal

Each diffracted wave will have its own phase

Highly simplified explanation: there is <u>much more</u> to this, but this conveys the idea

- **In fact, it is because each diffracted wave represents a different solution to the Schrödinger Eqn. for the electron in the crystal**
    - Resulting phase depends on the strength & spacing of the periodic potential of the lattice along a given direction in the crystal

High-resolution EM
general idea



So, appears "simple" enough …

(1) Calculate the phase differences for the different diffracted waves (not easy, but do-able)

(2) Create an interference pattern from the overlap of these phases in two-dimensions

High-resolution EM

general idea

Not even this "simple"

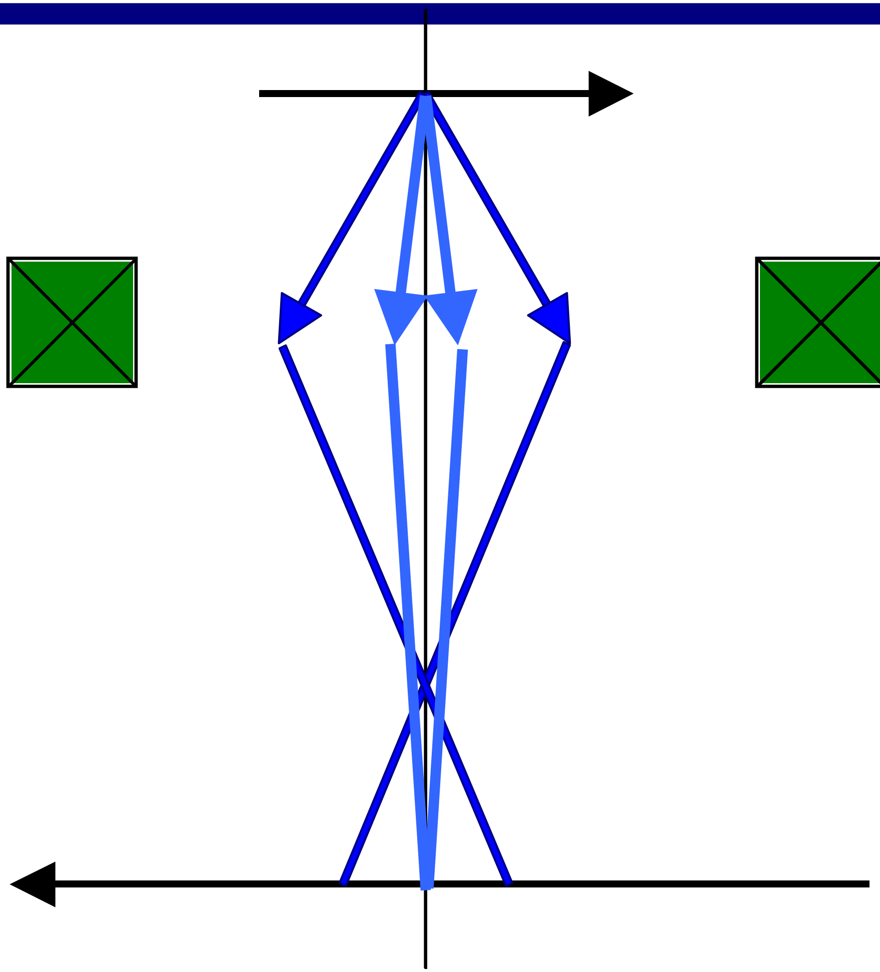
The TEM has very poor lenses

- Spherical aberration in particular

This aberration causes diffracted waves to be 'phase shifted' by the objective lens

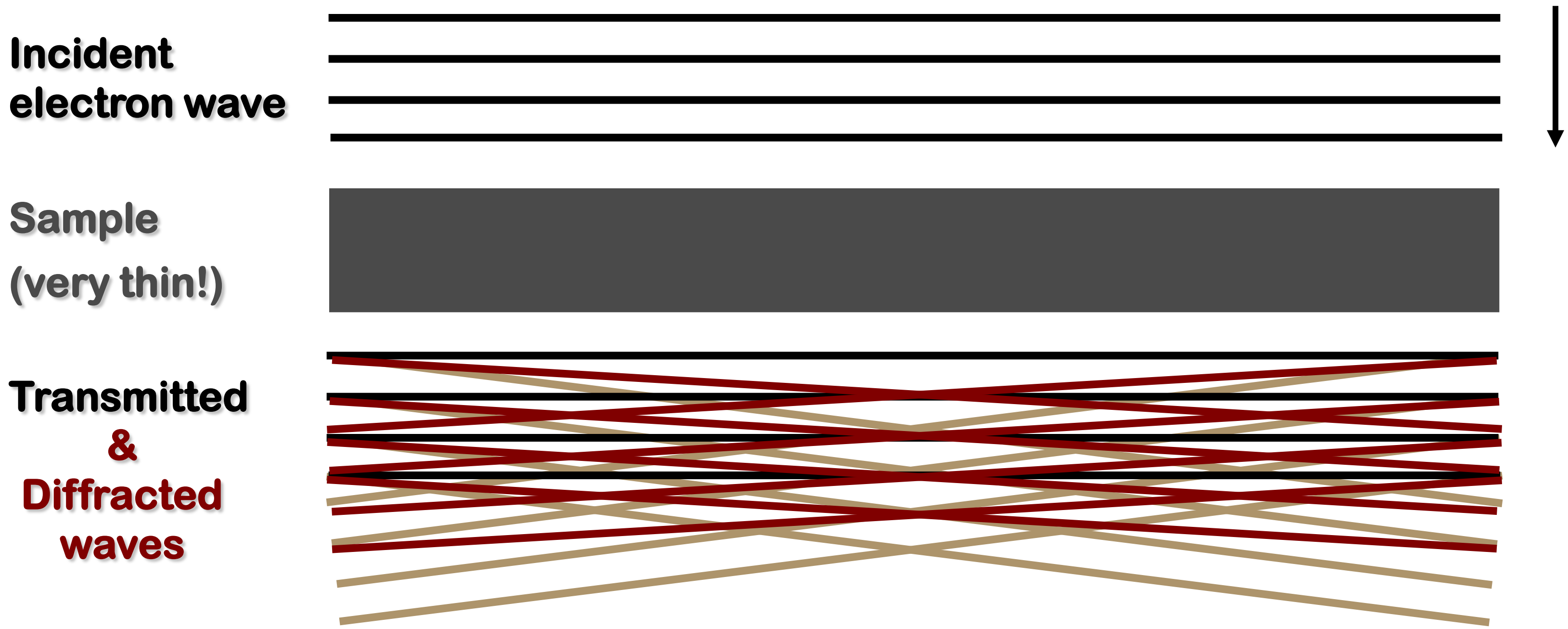
- Complex dependence on wavelength, C_s, diffraction vector and defocus
- Magnitude of phase shift varies with distance from optic axis
  - And thus diffraction angle
  - Thus each diffracted wave undergoes a different phase shift

Complicates image interpretation



Spherical aberration

High-resolution EM
general idea



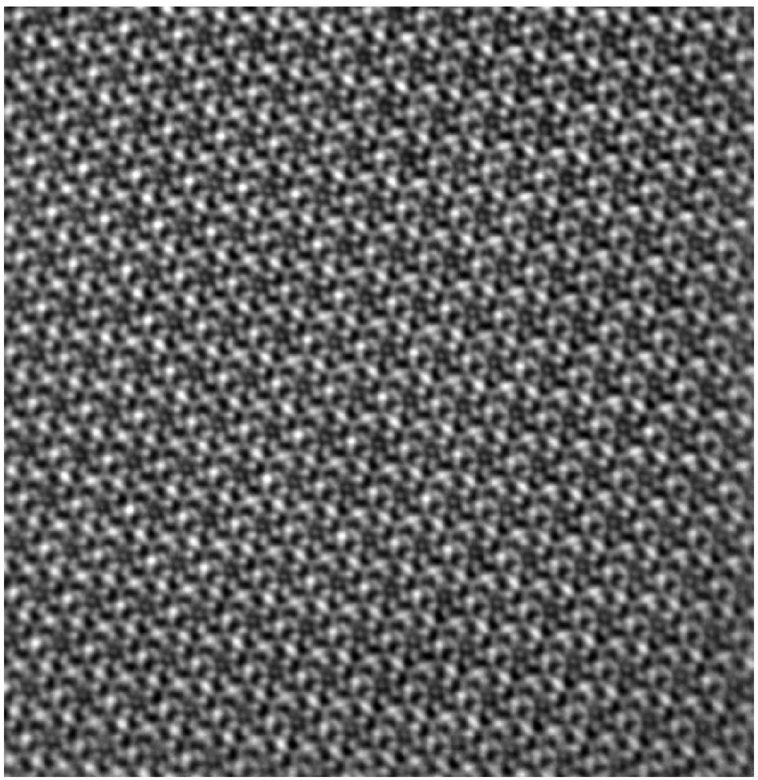
Returning to this picture

This means that the phases of the diffracted waves are changed by the objective lens focus

High-resolution EM
general idea

Thus, the image you get STRONGLY DEPENDS ON THE FOCUS CONDITION

A single HREM image



The 'unscrambled' exit wave

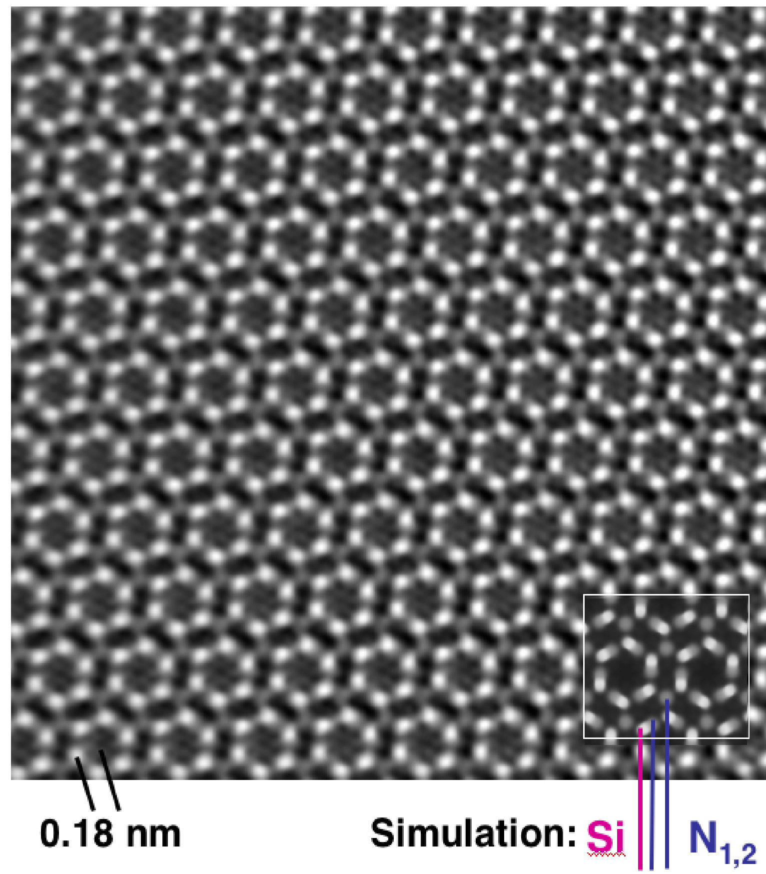


Image courtesy C. Kisielowski, NCEM, LBNL

High-resolution EM
general idea

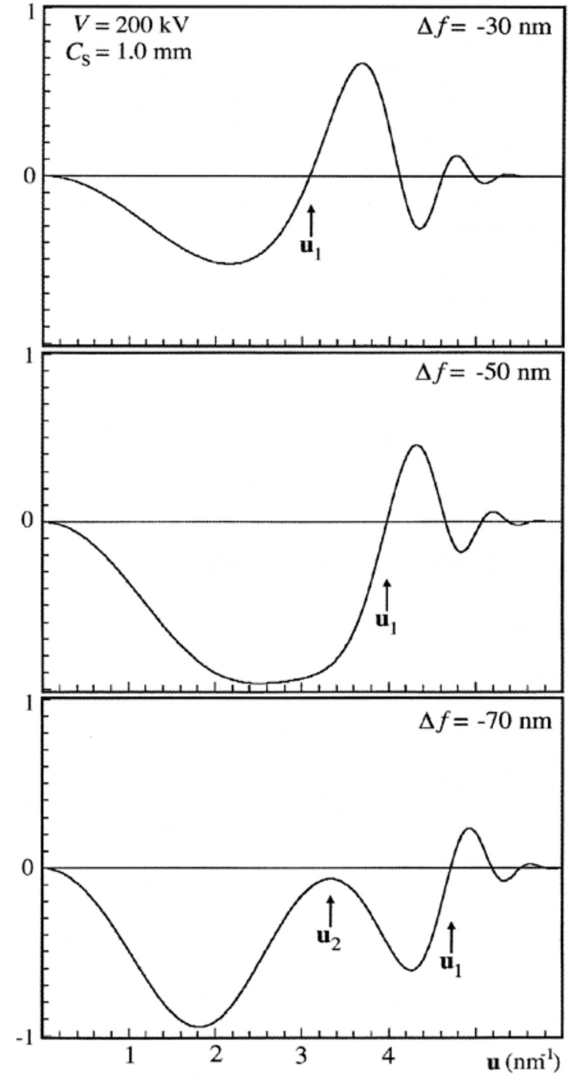
So, the lens effectively 'scrambles' the information embedded in the exit wave

The amount of scramble depends on the defocus & C_s

Embodied in the 'Contrast Transfer Function'

Different diffracted waves undergo different modifications of their spatial frequencies

"relative information transfer"



Inverse d-spacing of the reflection

Scherzer defocus

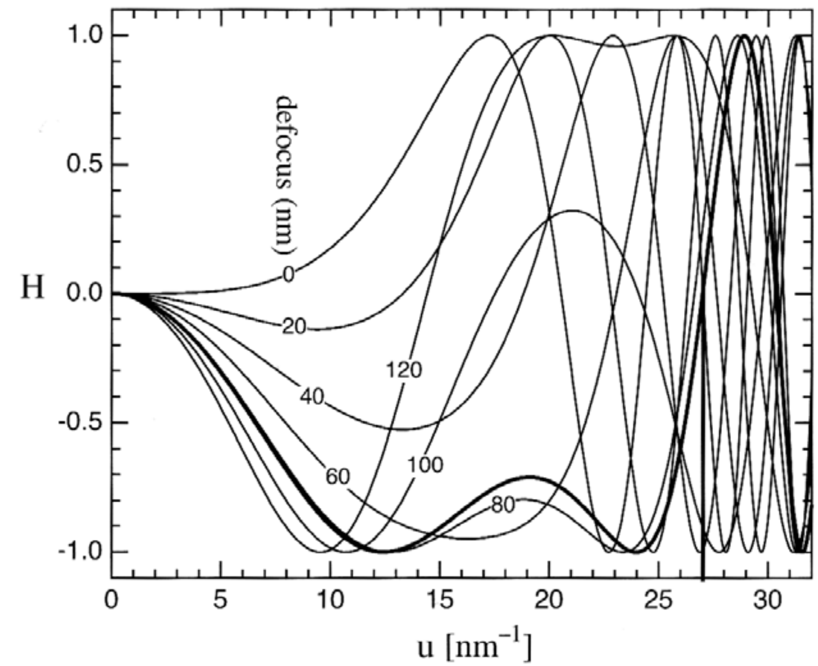
Balance effect of spherical aberration with a specific value of negative defocus.

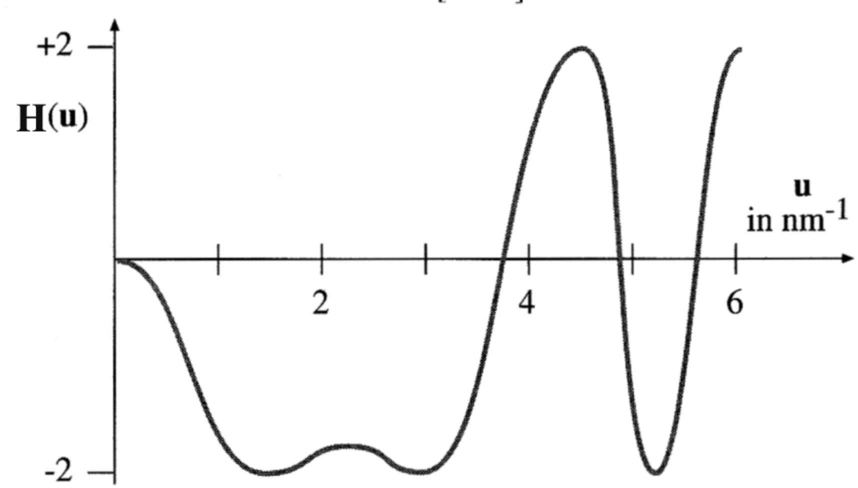
Scherzer defocus:

$$\Delta f = -\left(\frac{4}{3} C_s \lambda\right)^{1/2}$$

Scherzer resolution:

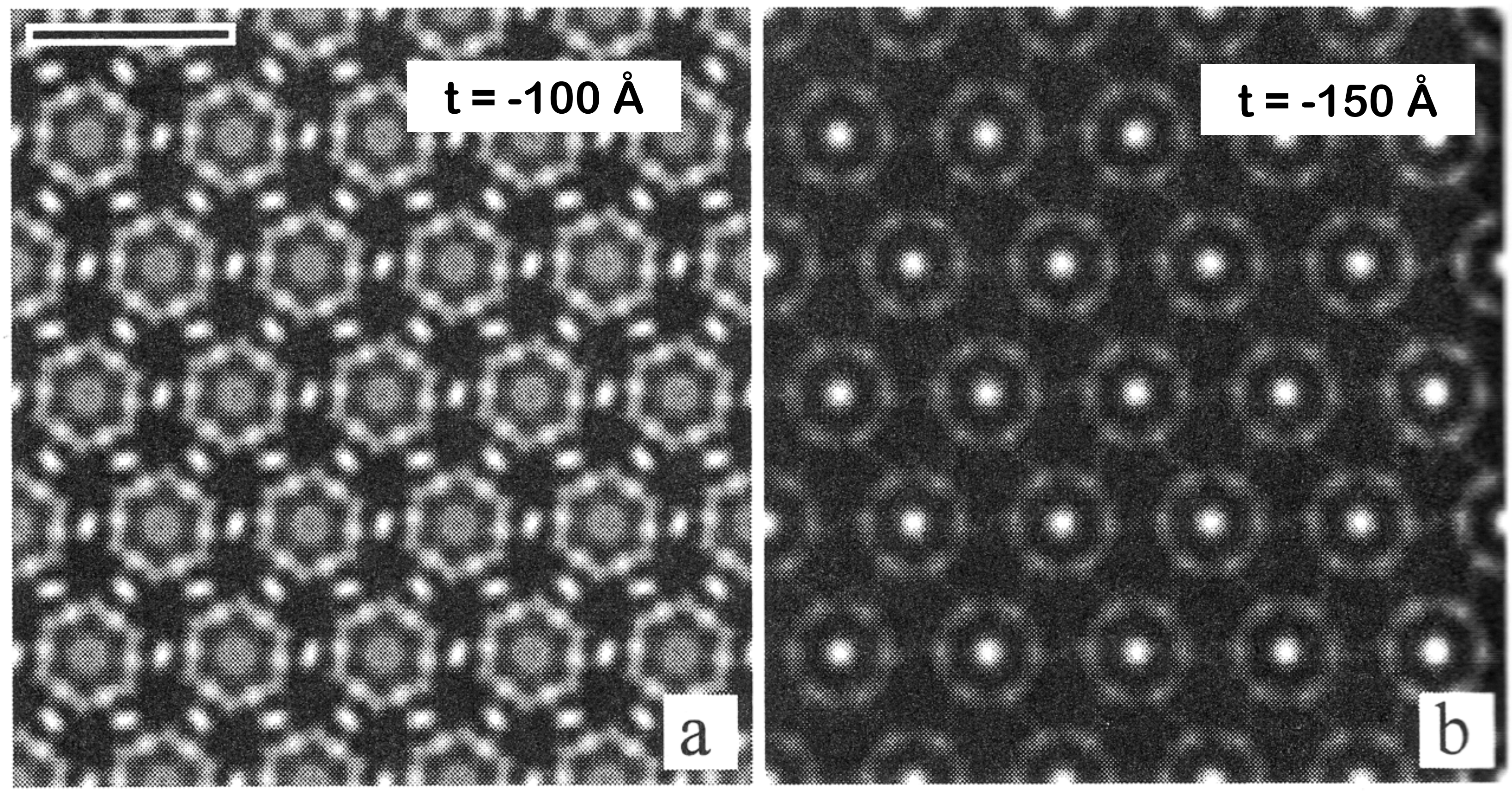
$$R_{Scherzer} = \frac{1}{1.51} C_s^{-1/4} \lambda^{-3/4}$$





Example

Si_3N_4 (0001)



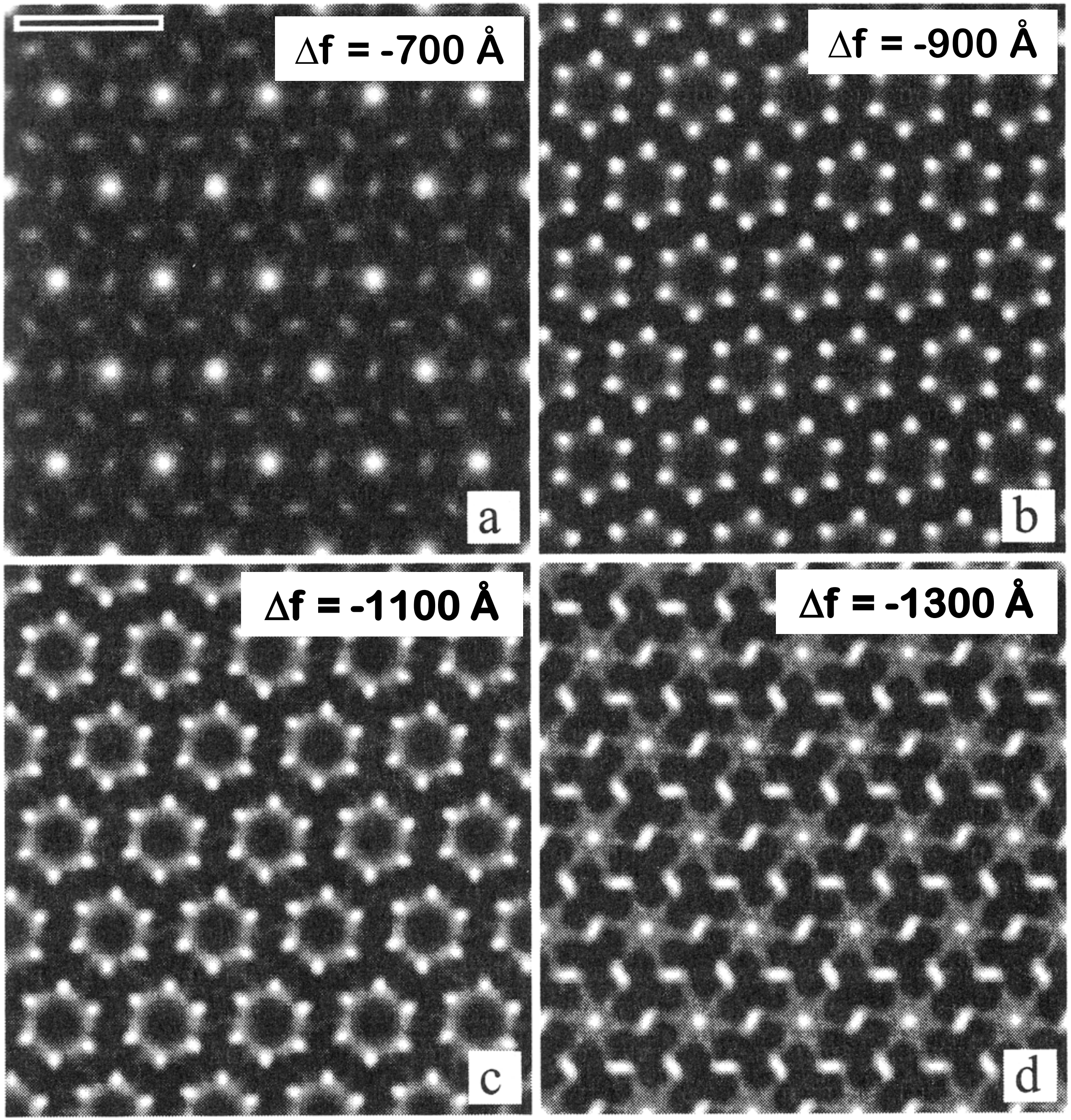
Images depend on sample thickness

(different phase shift as electron wave travels a different distance)

From E.J. Kirkland, *Advanced Computing in Electron Microscopy*

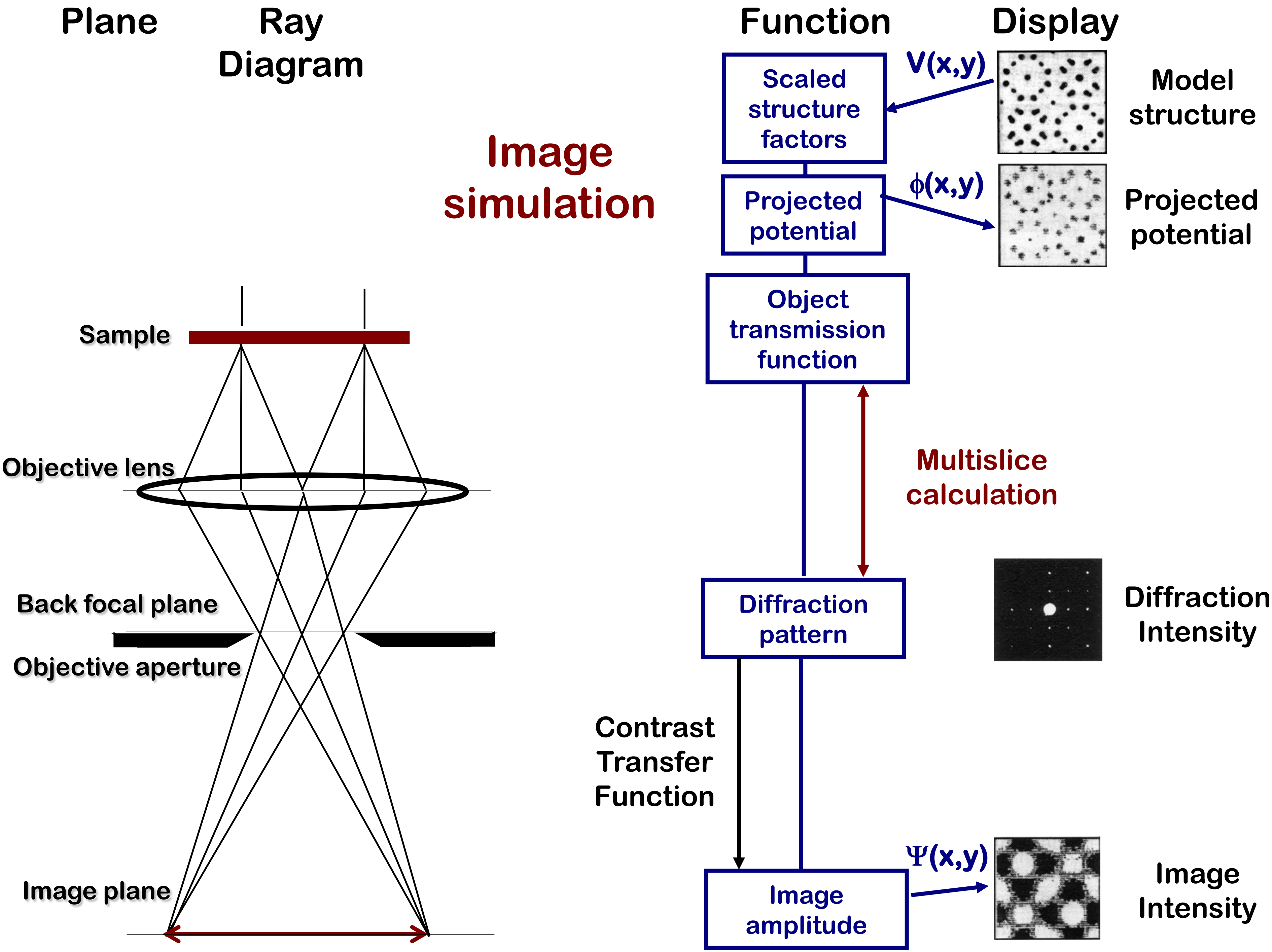
Example

Si_3N_4 (0001)



Images depend on focus

Different relative phases shifts of the diffracted waves with respect to the transmitted wave



Plane
Ray Diagram
Function
Display
Image simulation
Scaled structure factors
V(x,y)
Model structure
Projected potential
ϕ(x,y)
Projected potential
Object transmission function
Multislice calculation
Diffraction pattern
Diffraction Intensity
Contrast Transfer Function
Image amplitude
Ψ(x,y)
Image Intensity
Sample
Objective lens
Back focal plane
Objective aperture
Image plane

Summary - HRTEM

Image strongly depends on defocus

Relationship between image and "atomic positions" is not straightforward

Understanding of imaging conditions (via defocus, sample thickness and microscope calibrations) necessary

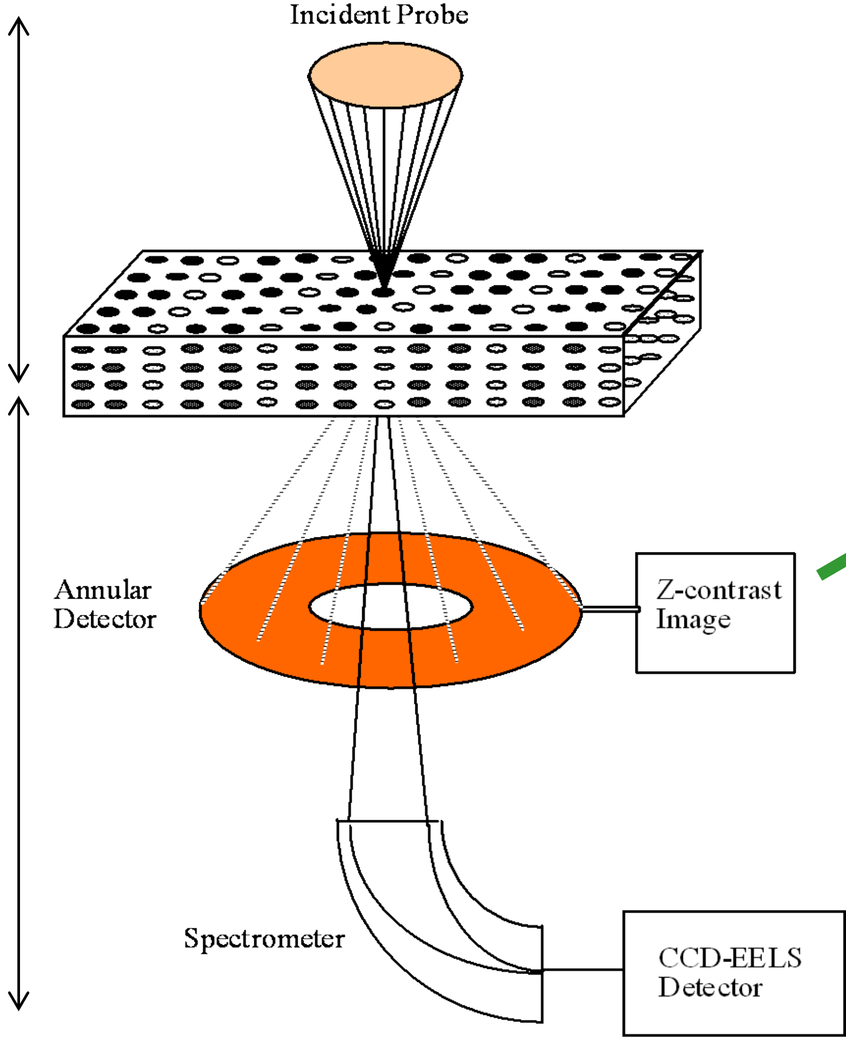
These provide inputs for image simulation

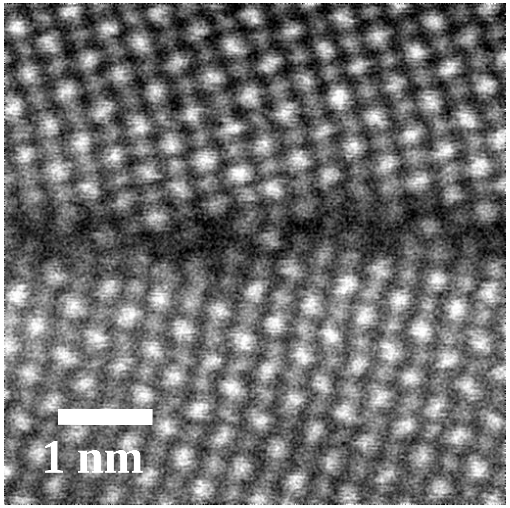
Proper match of the image with the calculation required for true understanding of the image

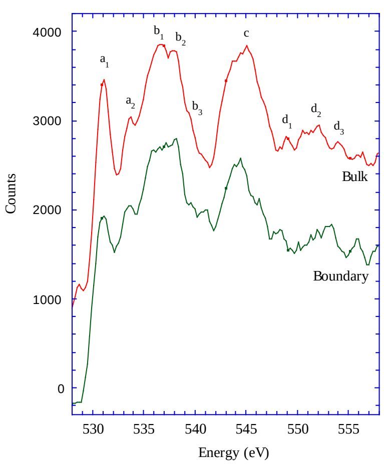
STEM
general idea

Resolution

Image Properties







Courtesy Nigel Browning

Types of STEM images

Bright-field

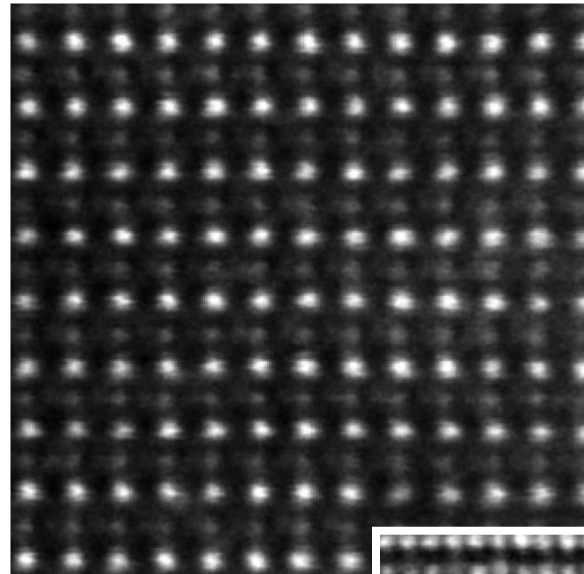
- Collect central beam with a small collection angle
- Contains elastic (Rutherford), phonon, plasmon and Compton

Low-angle annular dark field

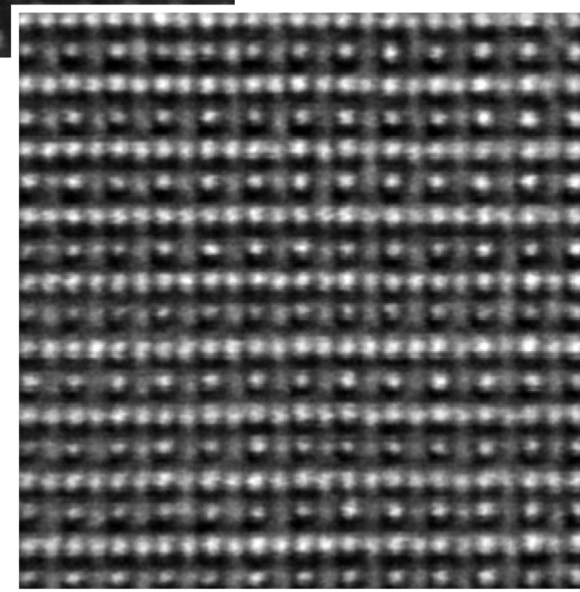
- Collection angle of 25 - 50 milliradians (mrad)
- Mostly phonon scatter

High-angle annular dark field

- Collection angle of 50 - 250 mrad
- Largely phonon scatter (TDS)



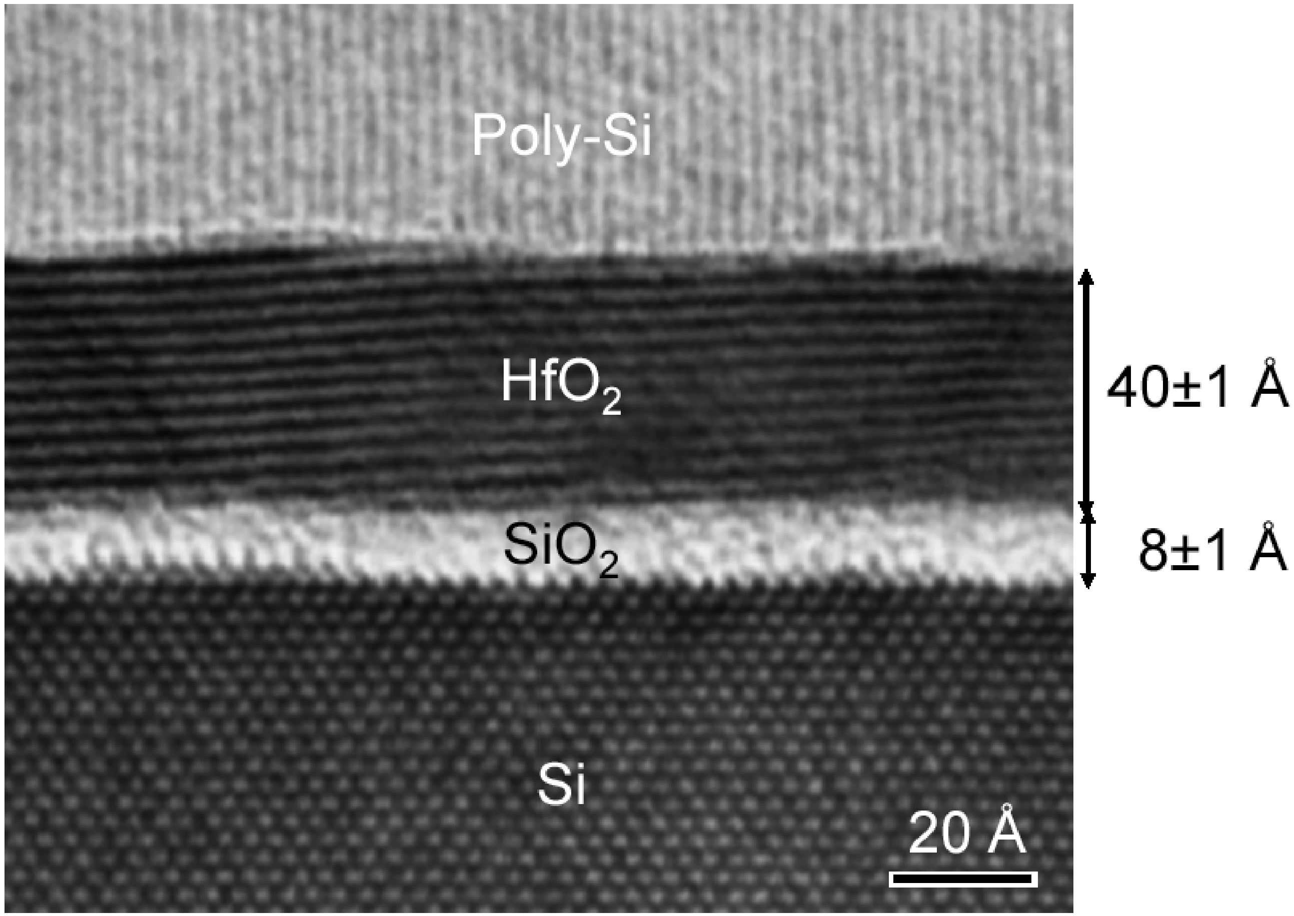
Coherent BF-STEM image of $SrTiO_3$ <110>



HAADF-STEM

Images from S.J. Pennycook

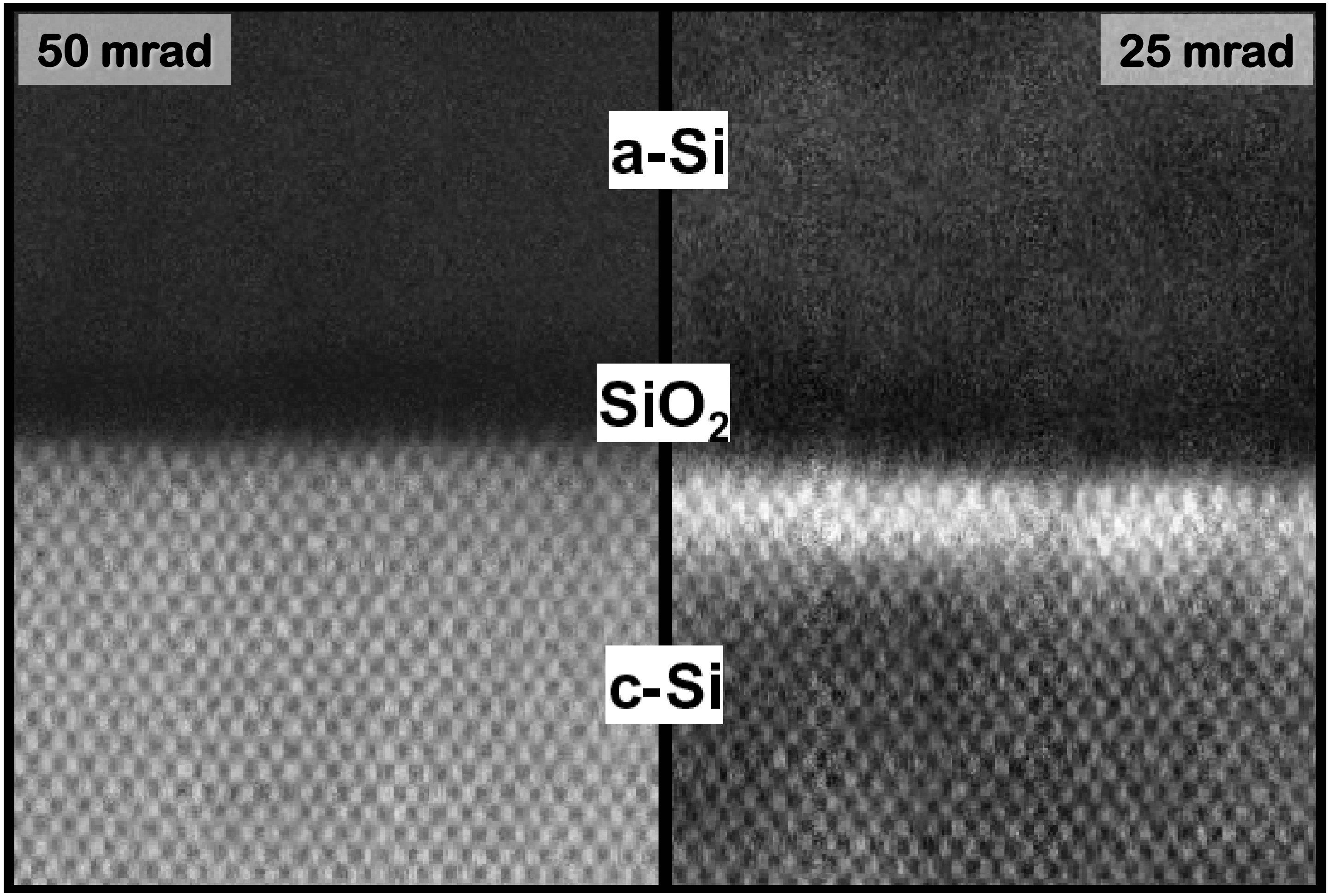
BF-STEM



"Reciprocity" with HRTEM images

Images courtesy Dave Muller

Low-angle annular dark field (LAADF)



Strain fields cause de-channeling and scattering to small angles

Images courtesy Dave Muller

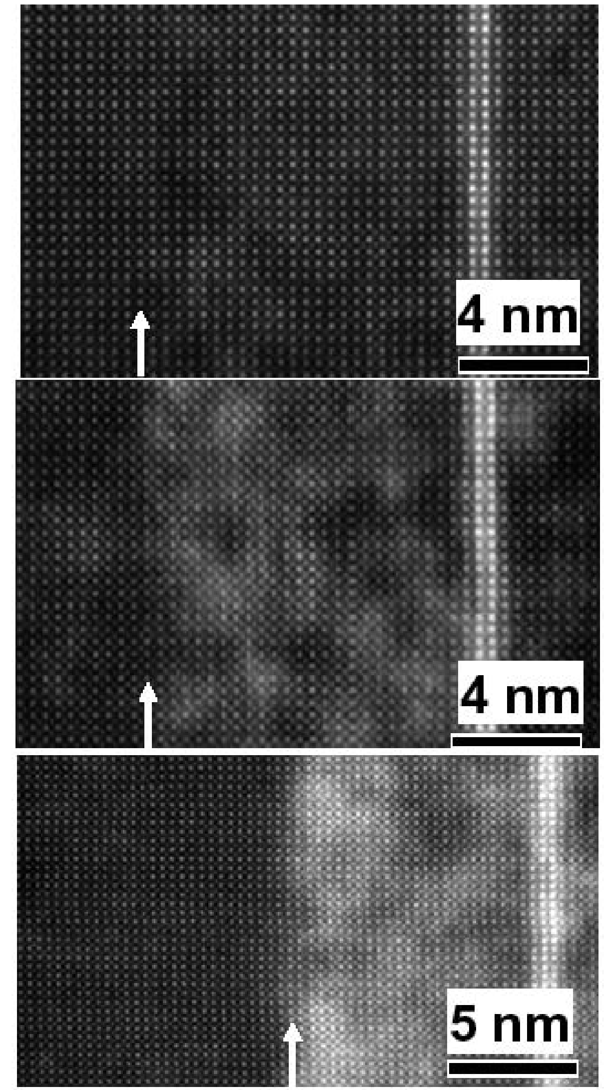
Low-angle annular dark field (LAADF)

Here contrast is correlated with oxygen vacancies

HAADF
"Z" map

LAADF
"Strain" map
Thin x/s

LAADF
"Strain" map
Thick x/s



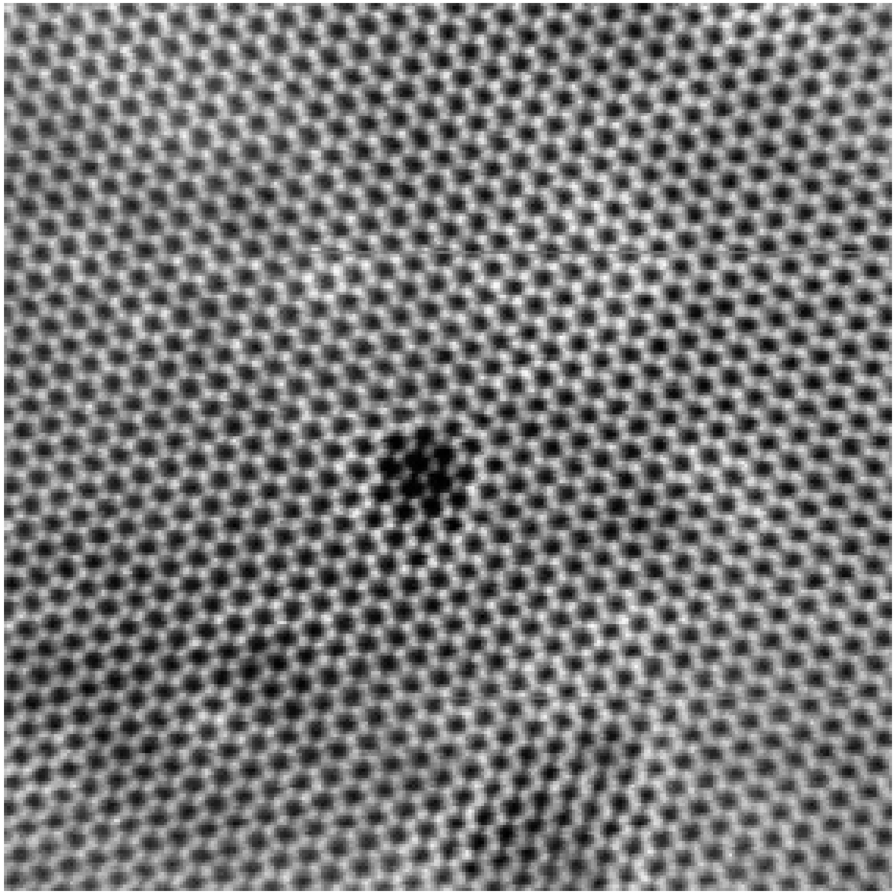
Images courtesy Dave Muller

High angle annular dark field (HAADF)

No contrast reversals with thickness

Directly 'interpretable' images

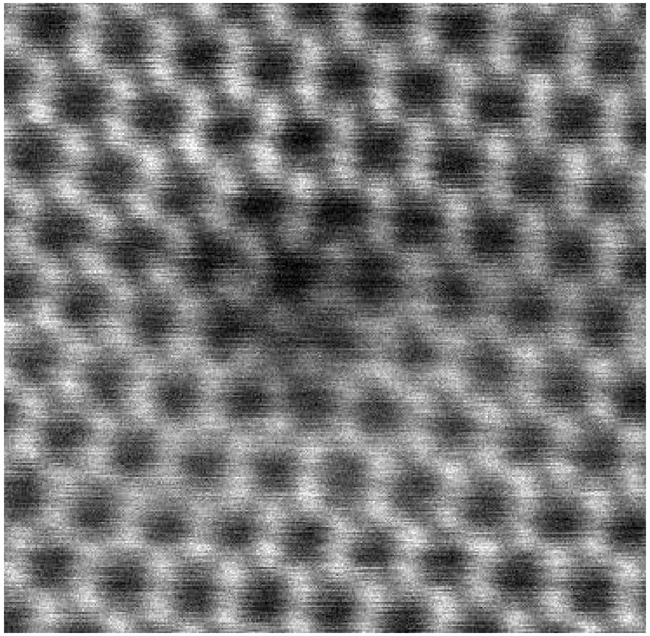
- If you see a white blob, there's an atom column there
- Caveat: the person taking (& processing) the image knew what they were doing …

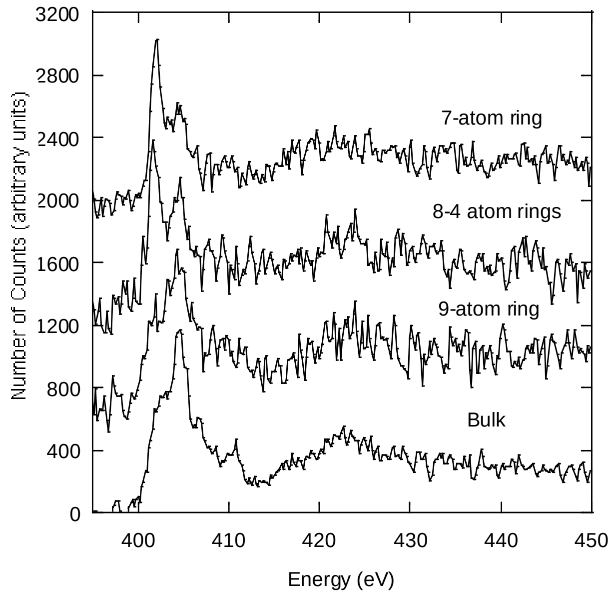


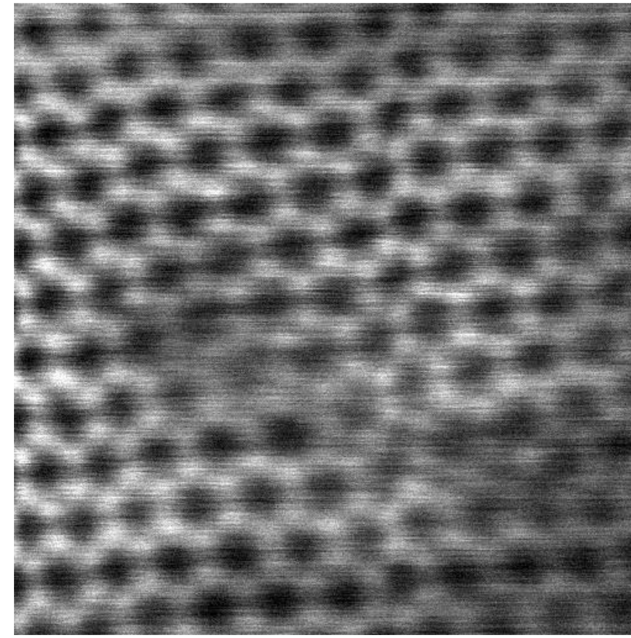
Screw dislocation core in GaN

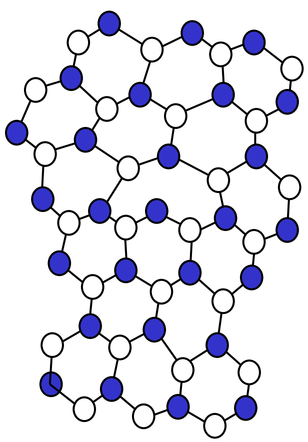
Image courtesy Ilke Arlsan, Nigel Browning

HAADF of dislocation cores





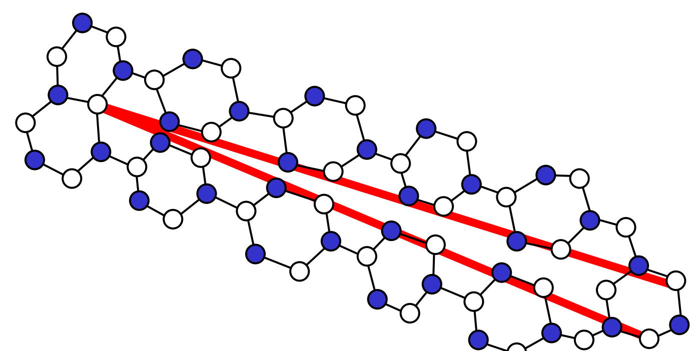




$$\frac{1}{3}[113] \rightarrow \frac{1}{3}[110] + [001]$$

or

$$\frac{1}{3}\left[11\bar{2}3\right] \rightarrow \frac{1}{3}\left[11\bar{2}0\right] + [0001]$$



Arslan, Bleloch, Stach and Browning, PRL 2005

Summary - STEM

Scatter to high angle is depended on atomic weight

Scanning a focused probe, combined with capturing this intensity can lead to an image that caries sensitivity to atomic weight differences

Can form atomic resolution images

– Directly interpretable

– Show atomically sensitive contrast

Can be combined with EELS to give spectroscopic information atomic column-by-atomic column