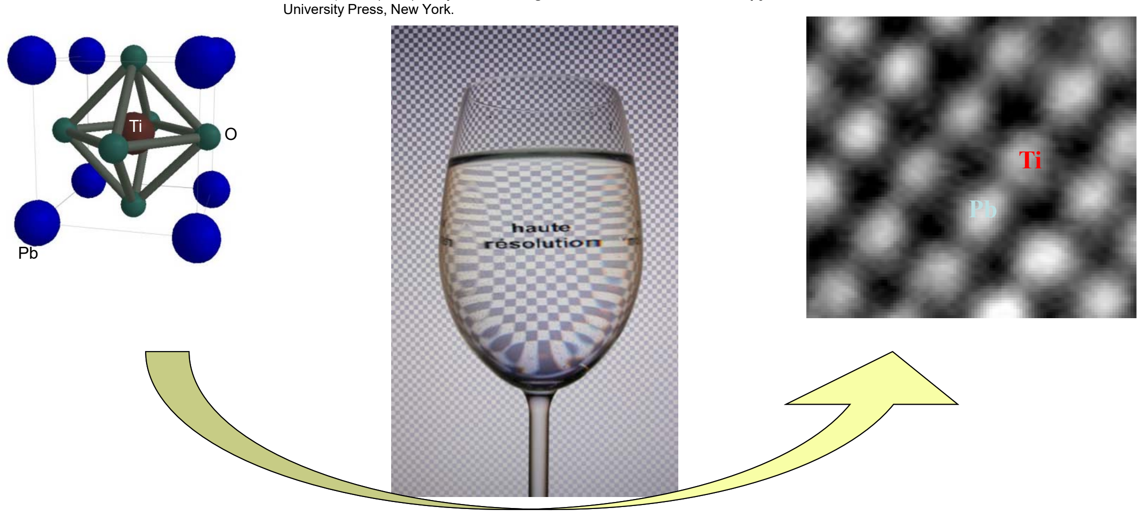
High Resolution TEM
without Cs corrected microscopes

- K. Ishizuka (1980) ***"Contrast Transfer of Crystal Images in TEM"***, Ultramicroscopy **5**,pages 55-65.
- L. Reimer (1993) ***"Transmission Electron Microscopy"***, Springer Verlag, Berlin.
- J.C.H. Spence (1988), ***"Experimental High Resolution Electron Microscopy"***, Oxford University Press, New York.



Abbé's principle in light optics

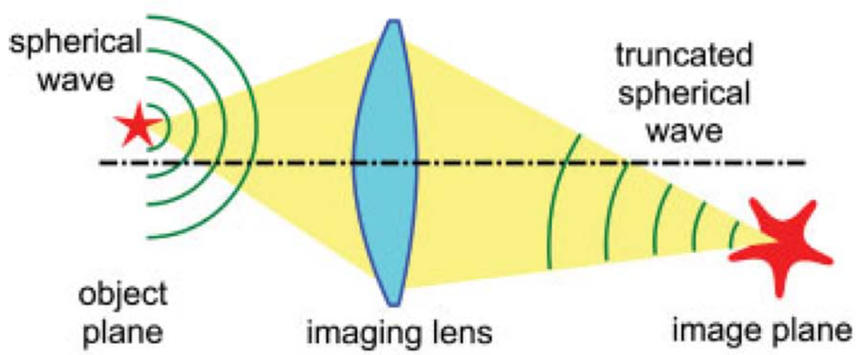
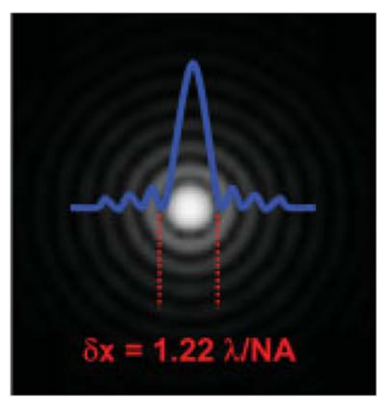


Figure 21-2: Image formation of self-luminous objects.



x: resolution (point spread function)
λ: wave length
NA: numerical aperture (lens diameter)

Handbook of Optical Systems: Vol. 2. Physical Image Formation.

Abbé: image formation by diffraction

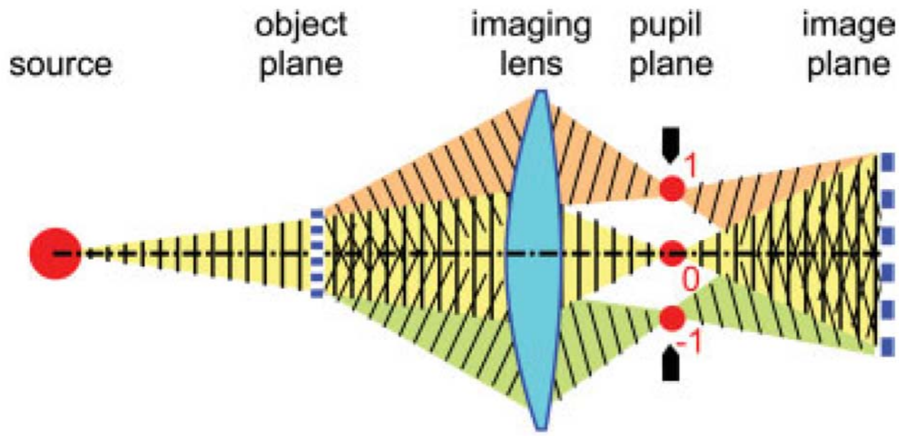
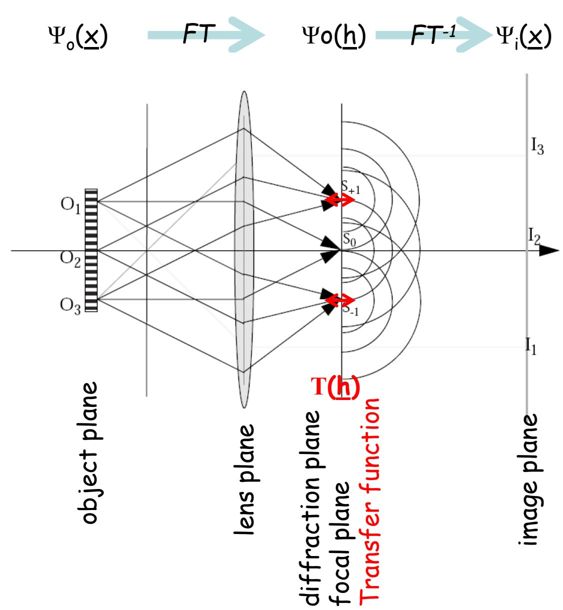


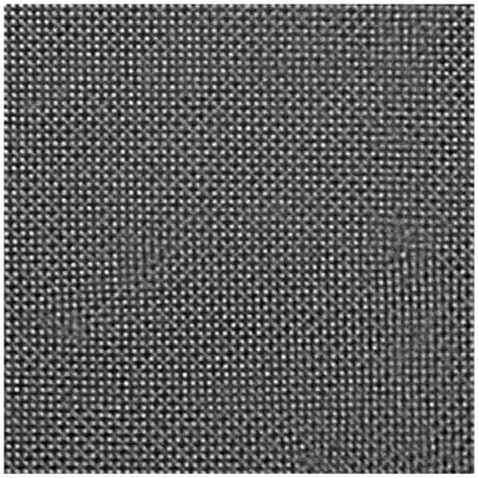
Figure 21-3: Abbe Theory of image formation by diffraction and interference.

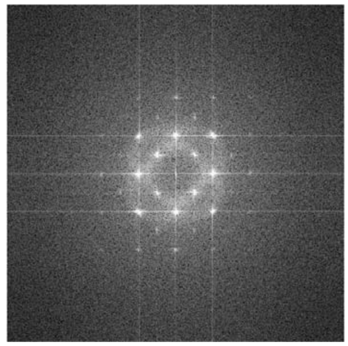
Abbé's principle of image formation

A lens is an analogous «light-speed fast» Fourier-Transformer

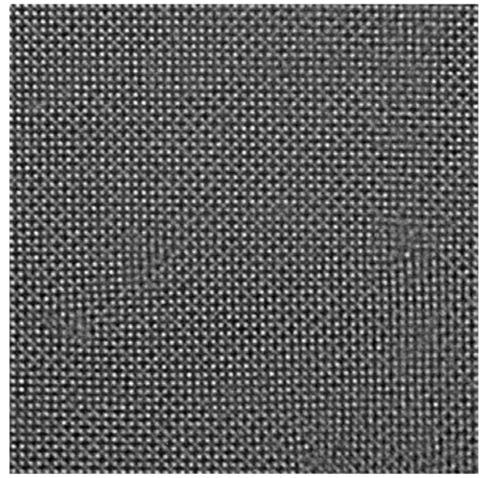


Abbé's principle mathematically



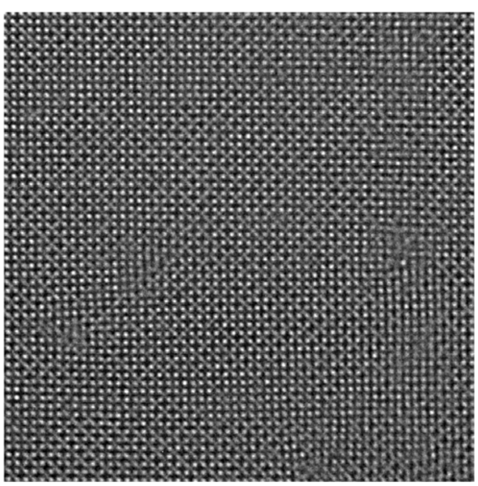


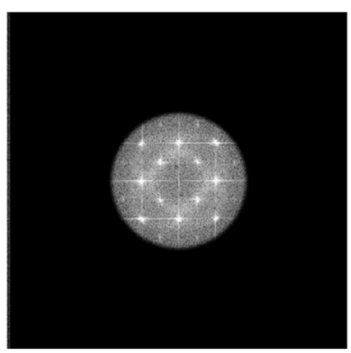
FFT



object $\xrightarrow{FT}$ $\xrightarrow{FT^{-1}}$ image

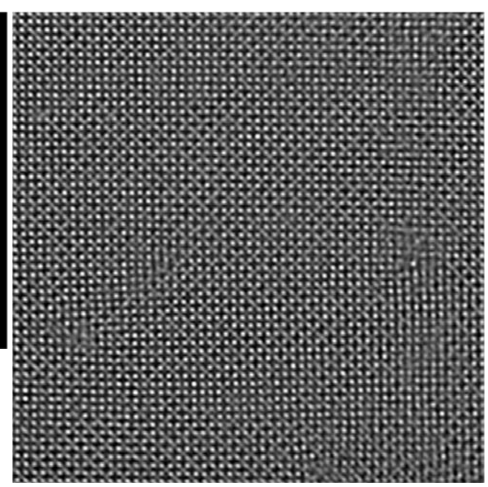
Abbé's principle mathematically



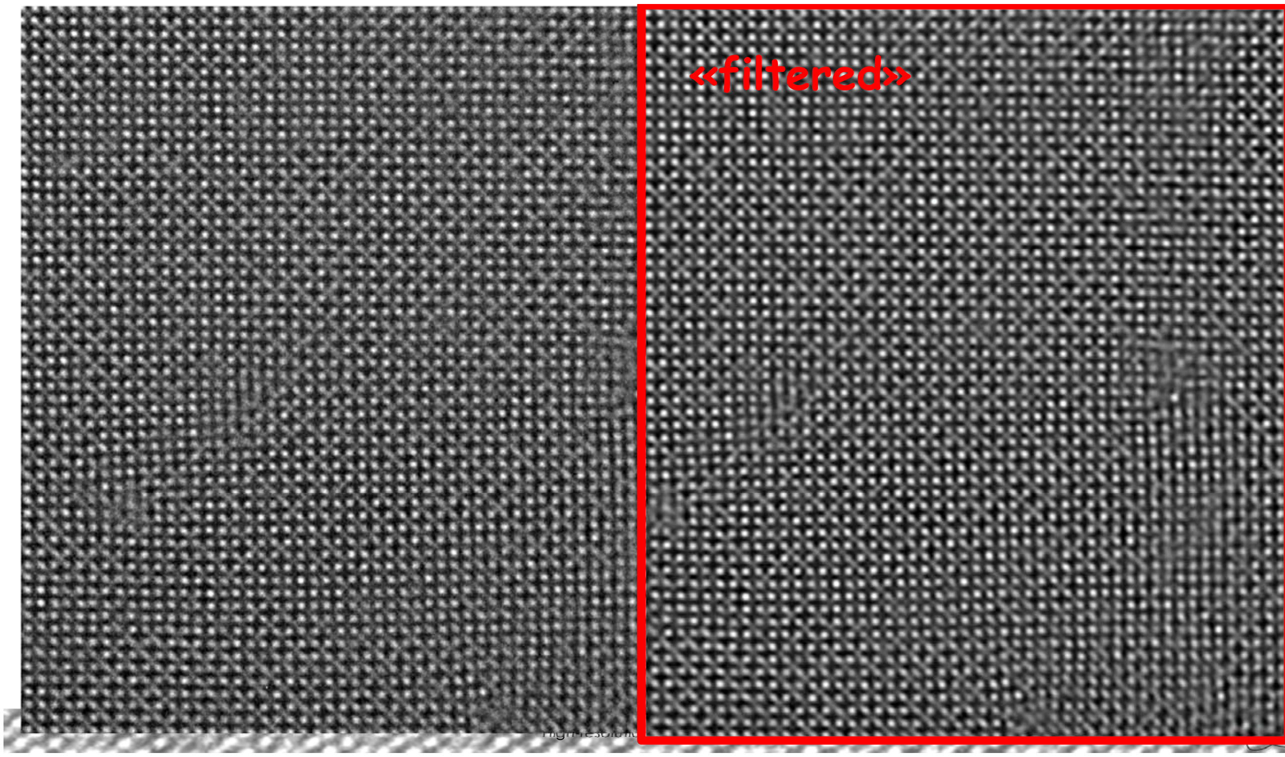


FFT

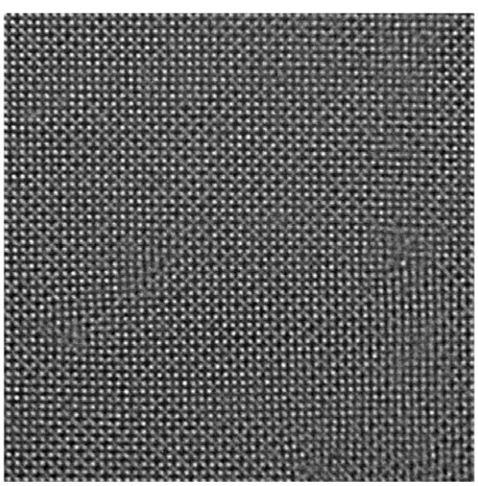
with mask

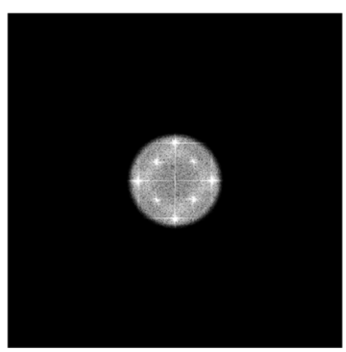


object $\xrightarrow{FT}$ $\xrightarrow{FT^{-1}}$ image

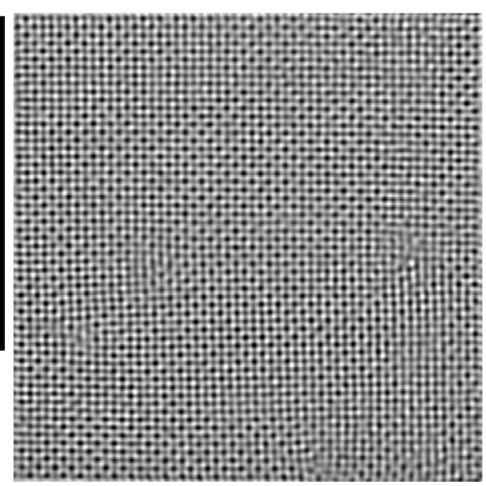


Abbé's principle mathematically



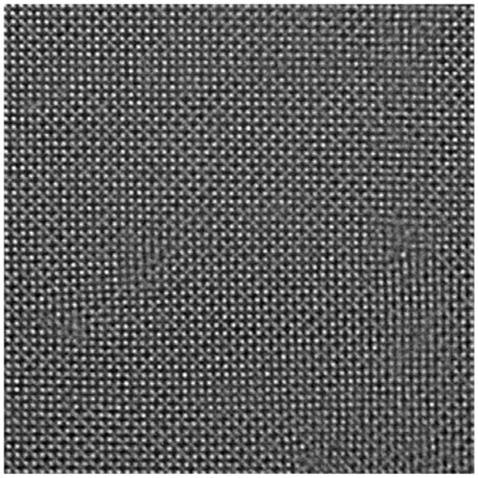


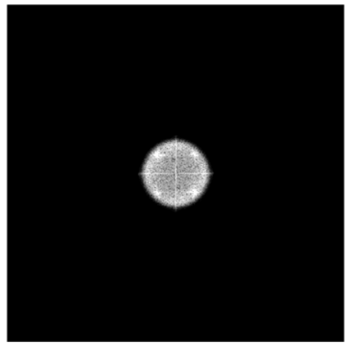
FFT



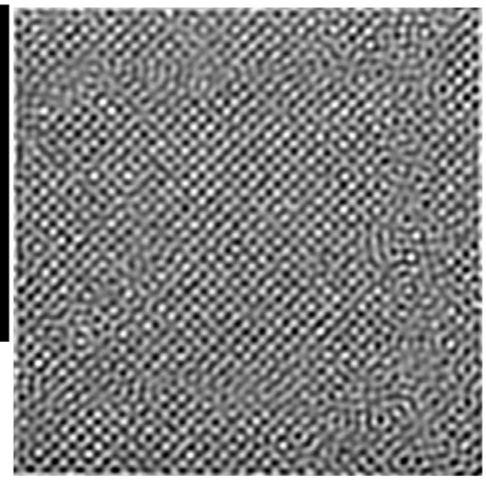
object FT FT^{-1} image

Abbé's principle mathematically



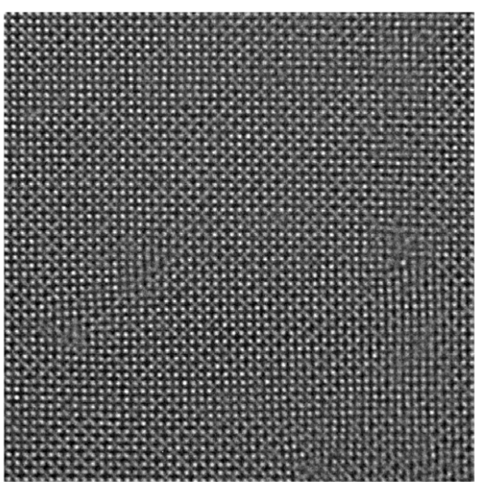


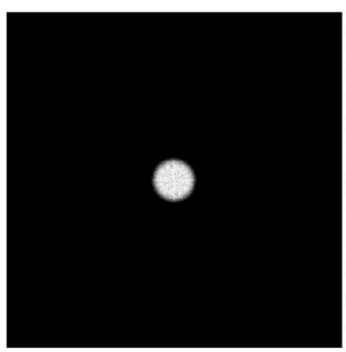
FFT



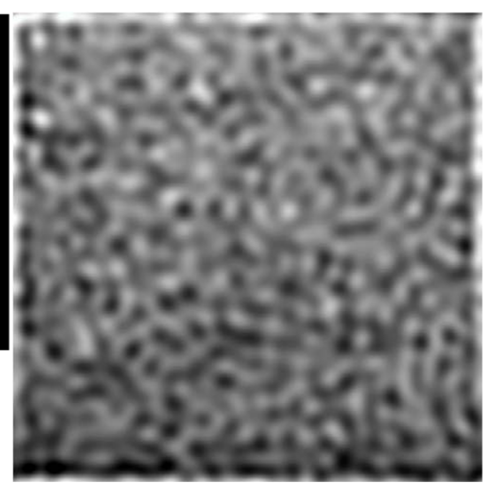
object FT → FT^{-1} → image

Abbé's principle mathematically





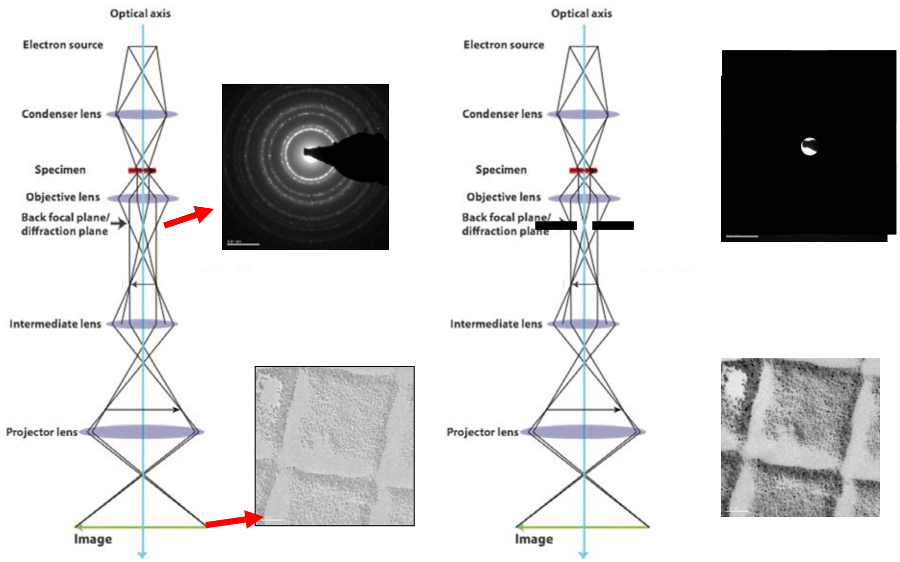
FFT

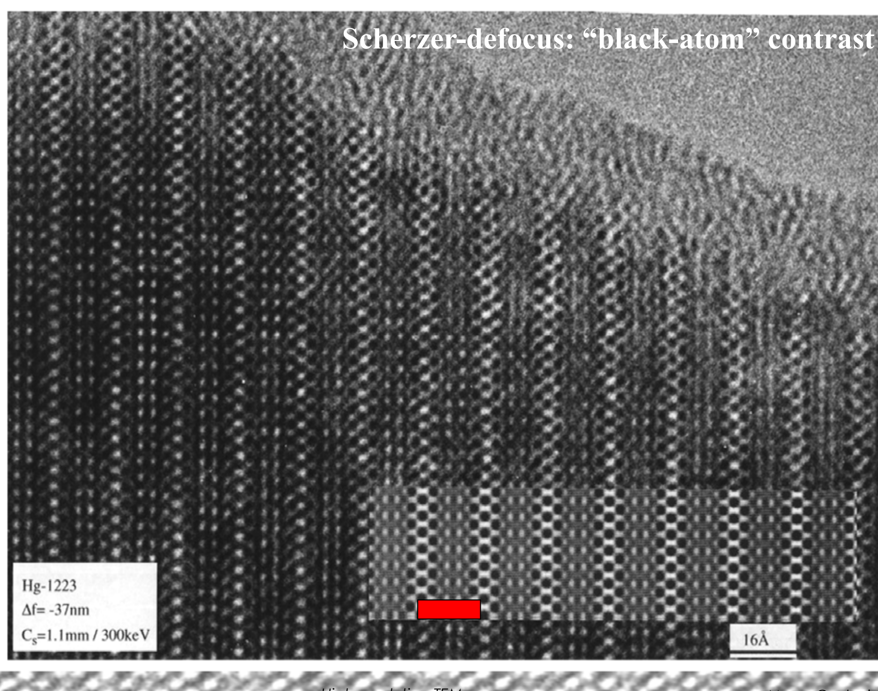


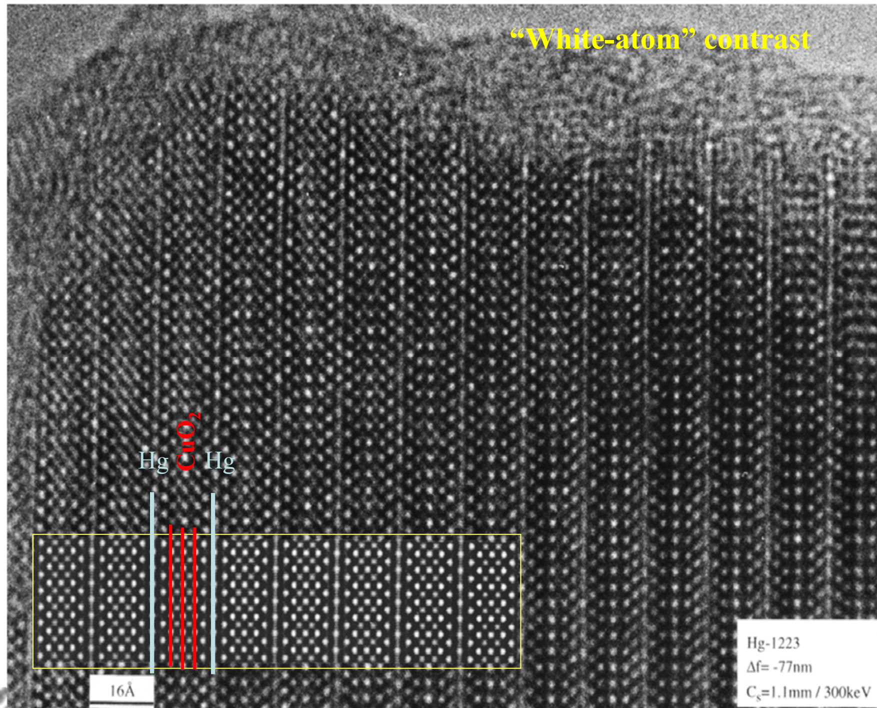
object FT → FT^{-1} → image

Bright Field Imaging

diffraction Contrast, Au (nano-) particles on C film







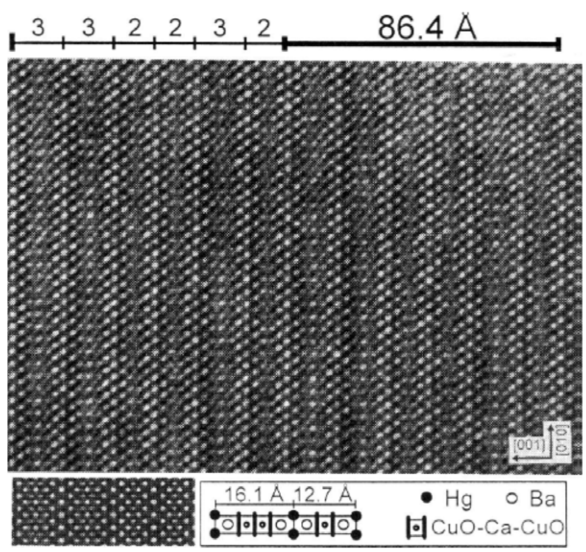
High-resolution

Expectation: The image should resemble the atomic structure !

Atoms…?
Thin samples: atom columns: orientation of the sample (incident beam // atom columns)

The observed contrast varies with thickness and defocalisation…!

Need to compare with simulations !

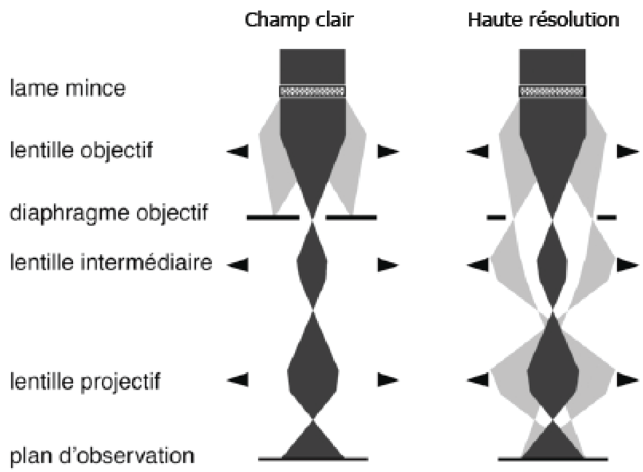


the TEM in "high-resolution" mode

A high-resolution image is an interference image of the transmitted and the diffracted beams!

Diffracted electrons: coherent elastic scattering
(the electrons have seen the crystal lattice)

The quality of the image depends on the optical system that makes the beams interfere



Bright Field High-Resolution

the objective lens

Field with rotational symmetry

Lorentz Force : $\mathbf{F} = -e\,\mathbf{v} \wedge \mathbf{B}$

e on optical axis: $\mathbf{F} = 0$, e not on optical axis : deviated

optical axis: symmetry axis

Scherzer 1936:

Magnetic lens with **rotational symmetry**:

Aberration coefficients:

C_s: spherical

C_c: chromatical

Always positive !!

$$C_s = \frac{1}{16}\int_{z_o}^{z_i}\left\{b^4h^4 + 2(hb' + h'b)^2 h^2 + 2b^2h^2h'^2\right\}dz$$

$$C_c = \frac{1}{4}\int_{z_o}^{z_i} b^2h^2 dz$$

« Scherzer » resolution limit: $D_{res} = 0.66\lambda^{3/4}C_s^{1/4}$

Example: Talos/Osiris
λ= 0.00197nm, C_s = 1.8 mm
D_{res} = 2.2 10^{-10} = 2.2Å

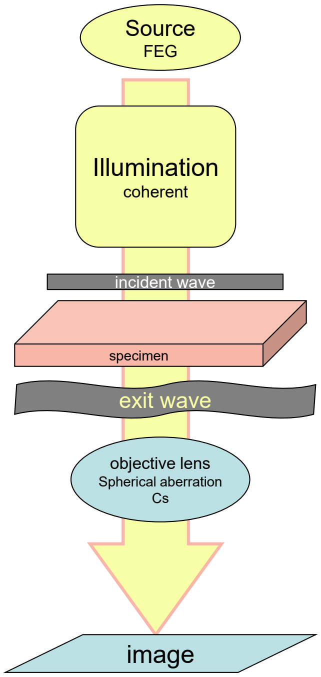


Image formation

- **Source:** *coherent and monochromatic*
- **Illumination:** *parallel*
- **Sample:** thin, *nicely prepared (no amorphization), orientation (zone axis)*
- **objective lens:** *aberrations, focus, stability !*
- **projection** lens system *(magnification)*

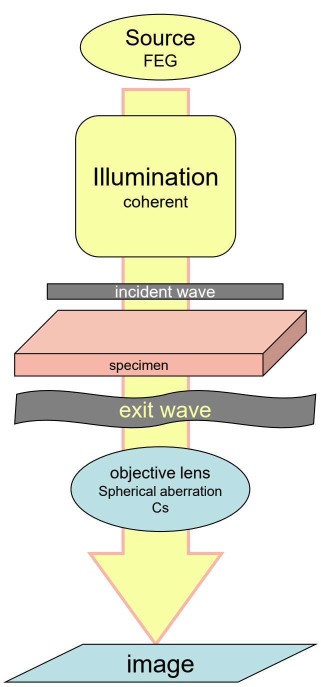


Image formation

- **Illumination:** *parallel beam*

$$\Psi(\vec{\mathbf{r}}) = \Psi_0 \exp^{2\pi i \vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}$$

- **Sample:**

  weak phase object:
  weak phase object aproximation (WPOA)

- **Objective lens:**

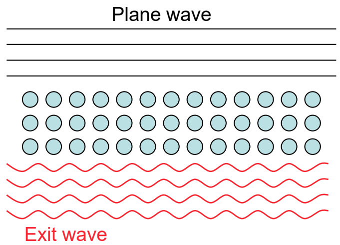
  Abbé's principle
  transfert function
  coherent transfer function (CTF)

$$\Psi_i(\vec{\mathbf{x}}) = \Psi_o(\vec{\mathbf{x}}) \otimes T(\vec{\mathbf{x}})$$

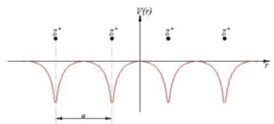
- **Image contrast** (intensity)

$$\mathrm{I}_\mathrm{i}(\vec{\mathbf{x}}) = \Psi_i(\vec{\mathbf{x}})\Psi_i^*(\vec{\mathbf{x}})$$

elastic scattering
sample = pure phase objet



Cristal potential



Cristal potential = phase object

Wave vector in vacuum:

$$k = \sqrt{2me(E) / h^2}$$

Wave vector in a potential:

$$k = \sqrt{2me(E + V(\vec{r})) / h^2}$$

Phase shift $\Delta\alpha$ due to the cristal potential V_p:

$$\Delta\alpha = \frac{\sigma}{2\pi} V_p(\vec{x}, z)$$

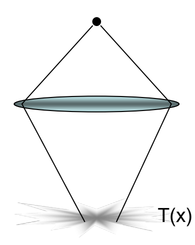
$$\sigma = \pi / \lambda E$$

Exit wave function: $\Psi_o(\vec{\mathbf{x}}) = exp\left[-i\sigma V_p(\vec{\mathbf{x}}; z)\right]$

Transfer Function

The optical system (lenses) can be described by a convolution with a transfer function T(x):
Point spread function (PSF): describes how a point on the object side is transformed into the image.

$$\Psi_i(\underline{x}) = \int_{-\infty}^{\infty} \Psi_o(\underline{u}) T(\underline{x} - \underline{u}) d\underline{u} = \Psi_o(\underline{x}) \otimes T(\underline{x})$$



- ***Transfer Function***:
  describe how a complex"object" wave-function is transfered into an "image" wave-function

$$\Psi_i(\underline{h}) = \Psi_o(\underline{h}) T(\underline{h})$$

- **The image INTENSITY** observed on a screen (or a camera / negative plate etc.)

$$I_i(\underline{x}) = \Psi_i(\underline{x}) \Psi_i^*(\underline{x})$$

$$I_i(\underline{h}) = \Psi_i(\underline{h}) \otimes \Psi_i^*(-\underline{h}) = \int \Psi_i(\underline{h}') \Psi_i^*(\underline{h} - \underline{h}') d\underline{h}'$$

$$I_i(\underline{h}) = [\Psi_o(\underline{h}) T(\underline{h})] \otimes [\Psi_o^*(-\underline{h}) T^*(-\underline{h})]$$

Transfer Function

$$T(\vec{\mathbf{h}}) = a(\vec{\mathbf{h}})\exp\left[2\pi i\chi(\vec{\mathbf{h}})\right]E_s(\vec{\mathbf{h}})E_t(\vec{\mathbf{h}})$$

- Phase factors:
  - Spherical Aberration
  - Defocus
- Amplitude factors:
  - (objective) apertures
  - spatial coherence enveloppe (non-parallel, convergent beam)
  - Temporal coherence envelope (non monochromatic beam, instabilities of the gun and lenses)

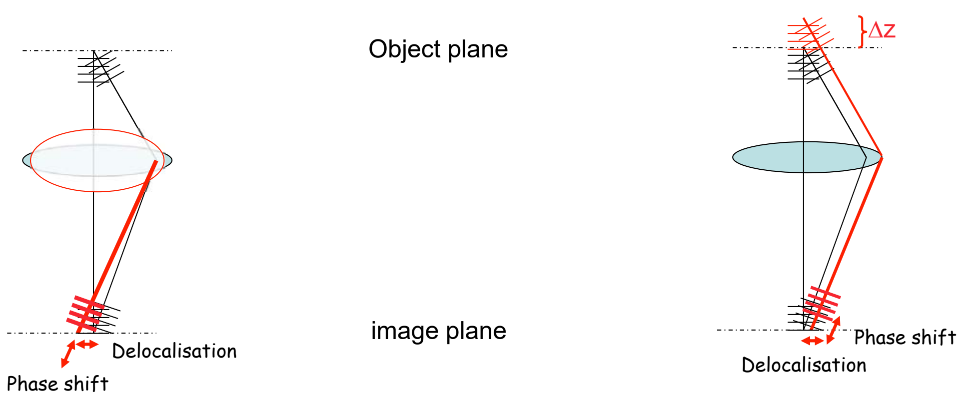
Transfer Function

$$T(\vec{\mathbf{h}}) = \exp\left[2\pi i\chi(\vec{\mathbf{h}})\right]$$

$$\chi(\vec{\mathbf{h}}) = 0.25C_s\lambda^3h^4 + 0.5\Delta z\lambda h^2$$

Spherical aberration

defocus



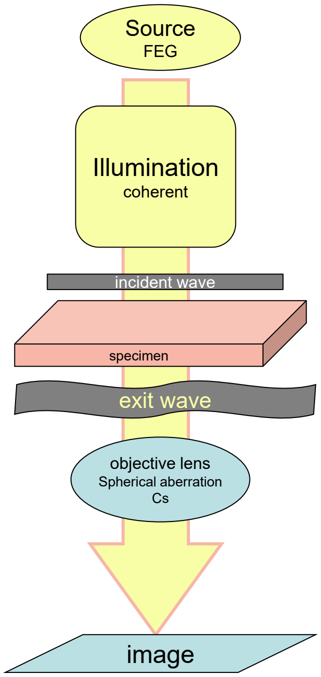


Image formation

- Illumination

$$\Psi(\vec{\mathbf{r}}) = \Psi_0 \exp^{2\pi i \vec{\mathbf{k}}\cdot\vec{\mathbf{r}}}$$

- Sample

$$\Psi_o(\vec{\mathbf{x}}) = exp\left[-i\sigma V_p(\vec{\mathbf{x}};z)\right] \cong 1 - i\sigma V_p(\vec{\mathbf{x}};z)$$

- objective lens

$$T(\vec{\mathbf{h}}) = \exp\left[2\pi i\chi(\vec{\mathbf{h}})\right] \quad avec \quad \chi(\vec{\mathbf{h}}) = 0.25C_s\lambda^3 h^4 + 0.5\Delta z\lambda h^2$$

$$\Psi_i(\vec{\mathbf{x}}) = \Psi_o(\vec{\mathbf{x}}) \otimes T(\vec{\mathbf{x}})$$

- Image, contrast

$$\mathrm{I_i}(\vec{\mathbf{x}}) = \Psi_i(\vec{\mathbf{x}})\Psi_i^*(\vec{\mathbf{x}})$$

The « magic » of image contrast

Weak phase object

$$\Psi_o(\underline{\boldsymbol{x}}) = exp[-i\sigma V_p(\underline{\boldsymbol{x}};z)] \cong 1 - i\sigma V_p(\underline{\boldsymbol{x}};z)$$

$$\Psi_o(\underline{\boldsymbol{h}}) = \delta(\underline{\boldsymbol{h}}) - i\sigma V_p(\underline{\boldsymbol{h}})$$

$$\Psi_i(\underline{\boldsymbol{h}}) = \Psi_o(\underline{\boldsymbol{h}})T(\underline{\boldsymbol{h}}) = \Psi_o(\underline{\boldsymbol{h}})exp[2\pi i\chi(\underline{\boldsymbol{h}})]$$

$$\Psi_i(\underline{\boldsymbol{h}}) = [\delta(\underline{\boldsymbol{h}}) - i\sigma V_p(\underline{\boldsymbol{h}})][\cos 2\pi\chi(\underline{\boldsymbol{h}}) + i\sin 2\pi\chi(\underline{\boldsymbol{h}})]$$

Fourier Space

Selecting $\sin[2\pi\chi(\underline{\mathbf{h}})] = -1$, $\cos[2\pi\chi(\underline{\mathbf{h}})] = 0$ ***for the strongest reflections*** $\underline{\boldsymbol{h}}$

Image wave function

$$\Psi_i(\underline{\boldsymbol{h}}) = \delta(\underline{\boldsymbol{h}}) - \sigma V_p(\underline{\boldsymbol{h}})$$

The image intensity $\Psi_i(\underline{\mathbf{x}})\,\Psi_i^*(\underline{\mathbf{x}})$) ***is given by :***

Intensity of a weak phase objet in "direct" contrast

$$I(\underline{\boldsymbol{x}}) = (1 - \sigma V_p(\underline{\boldsymbol{x}}))(1 + \sigma V_p(\underline{\boldsymbol{x}})) = \boxed{1 - 2\sigma V_p(\underline{\boldsymbol{x}})} + O(\sigma^2 V_p^2(\underline{\boldsymbol{x}}))$$

but….

Selecting $\sin[2\pi\chi(\mathbf{h})] = 0$, $\cos[2\pi\chi(\mathbf{h})] = 1$. *for the strongest reflections* ***h***

Image wave function

$$\Psi_i(\underline{h}) = [\delta(\underline{h}) - i\sigma V_p(\underline{h})]$$

Intensity of a weak phase objet in "reversed" contrast

$$I(\underline{x}) = (1 - i\sigma V_p(\underline{x}))(1 + i\sigma V_p(\underline{x})) = \boxed{1 + \sigma^2 V_p^2(\underline{x})}$$

Intensity is proportional to the square of the projected potential V_p : Image interpretation in terms of atom columns becomes complicated….

For a direct and simple interpretation of the image contrast:
the imaginary part (sin) of the transfer function exp[2πiχ(h)] should be ~-1

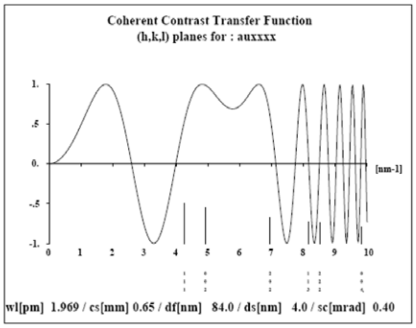
The only free parameter in the microscope is: the defocus Δz

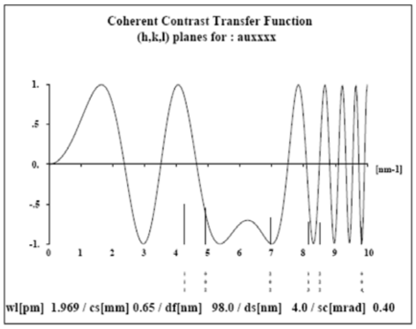
CTF

- CTF: contrast transfer function
  (« useful part » = V_p)

$$T(\vec{\mathbf{h}}) = \exp\left[2\pi i\chi(\vec{\mathbf{h}})\right]$$
$$\chi(\vec{\mathbf{h}}) = 0.25C_s\lambda^3h^4 + 0.5\Delta z\lambda h^2$$

$$CTF(h) = -\sin\left[\frac{\pi}{2}C_s\lambda^3h^4 + \pi\Delta z\lambda h^2\right]$$

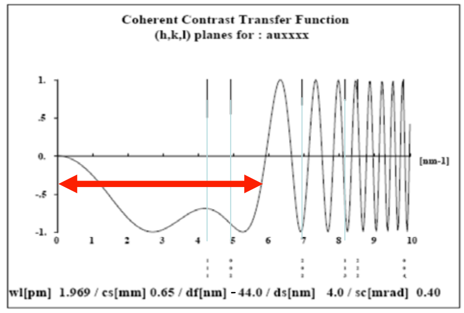




« Scherzer Defocus »

With $\Delta z_{scherzer}$

$$\Delta z = -\sqrt{{}^{4}/_{3}\, C_s \lambda}$$



The CTF has a wide pass band

$$D_{scherzer} = -0.66\lambda^{3/4} C_s{}^{1/4}$$

The first zero crossing of the CTF defines the « **point-to-point** » resolution of an electron microscope
The atom columns appear as dark areas on a bright background

$$I(\underline{x}) = (1 - \sigma V_p(\underline{x}))(1 + \sigma V_p(\underline{x})) = 1 - 2\sigma V_p(\underline{x}) + O(\sigma^2 V_p^2(\underline{x}))$$

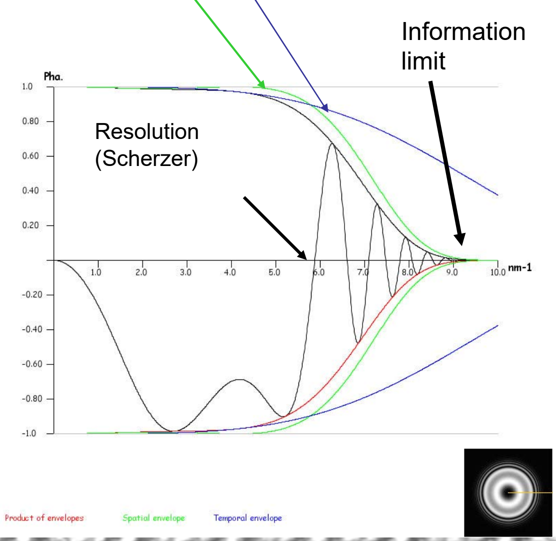
Spatial and temporal coherence

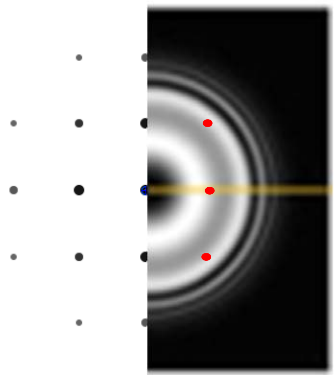
$$T(\vec{\mathbf{h}}) = a(\vec{\mathbf{h}}) \exp\left[2\pi i \chi(\vec{\mathbf{h}})\right] E_s(\vec{\mathbf{h}}) E_t(\vec{\mathbf{h}})$$

Fluctuations of lens current
Fluctuations of High Tension

CM300UT FEG
Field emission
C_s: 0.7mm
Dz= -44nm

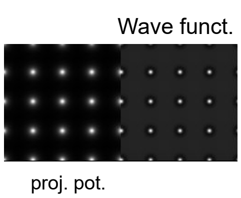
Resolution (point to point): 1.7Å
Information limit : ~1.2Å

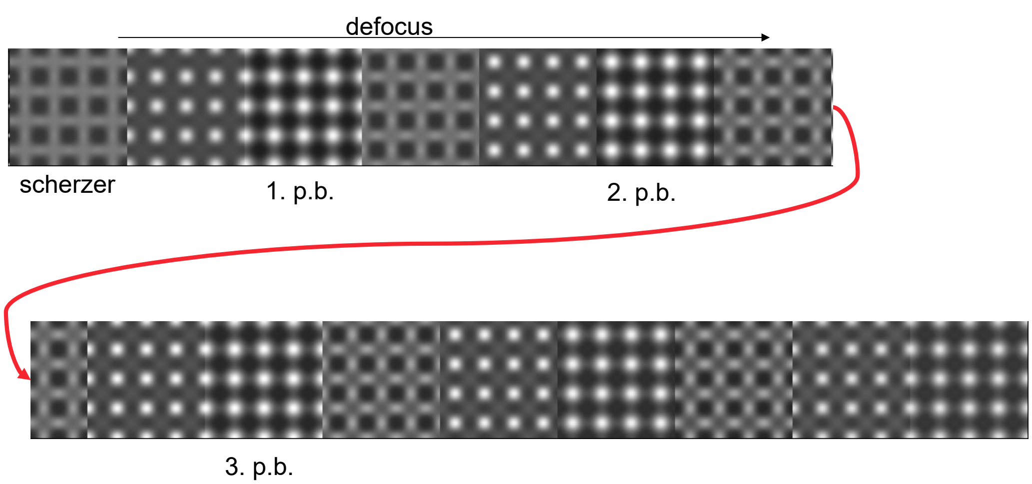


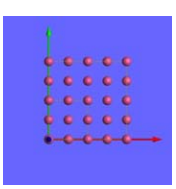


Back focal plane (diffraction plane)

Defocus

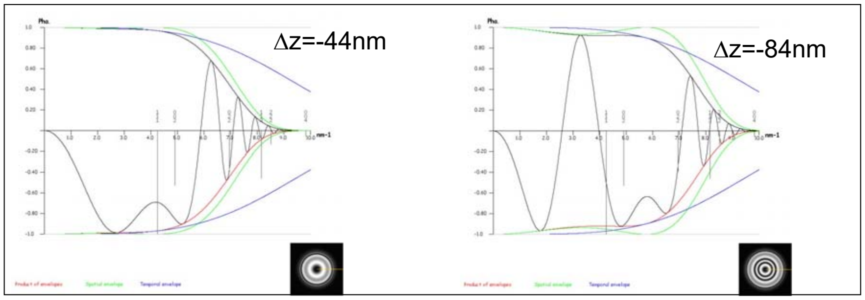






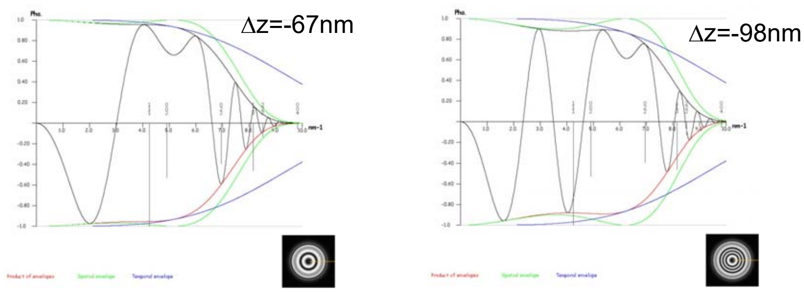
Au [100], thickness 20nm

Pass bands

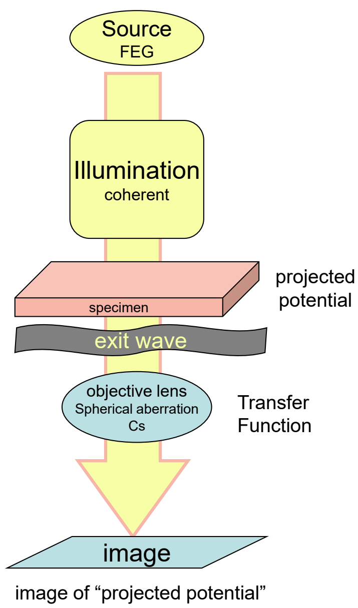


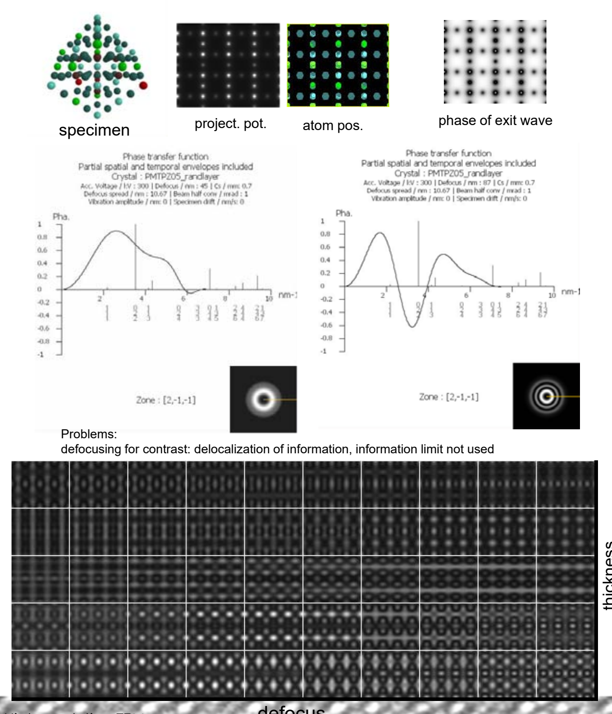
direct

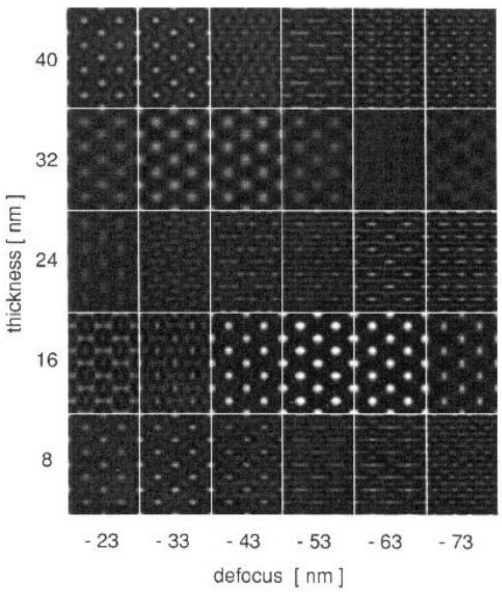
Réflexions hkl pour Au



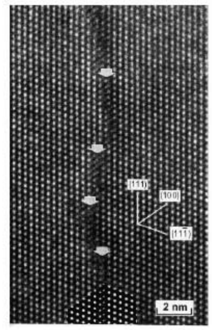
HRTEM image formation







Thickness-defocus map in Fe3Al intermetallics
M. Karlik Materials structure, 8 (2001),3

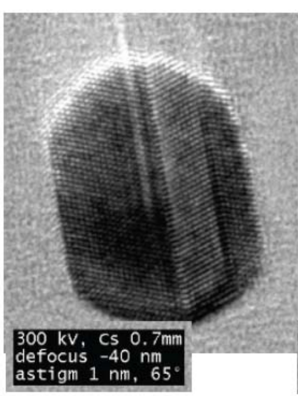


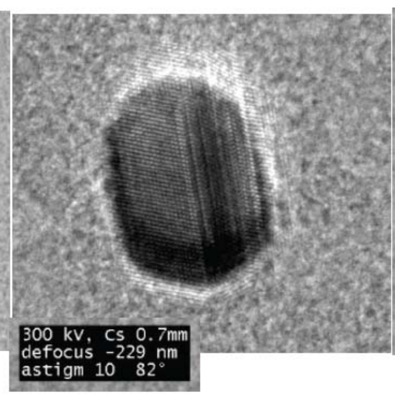
Experiment

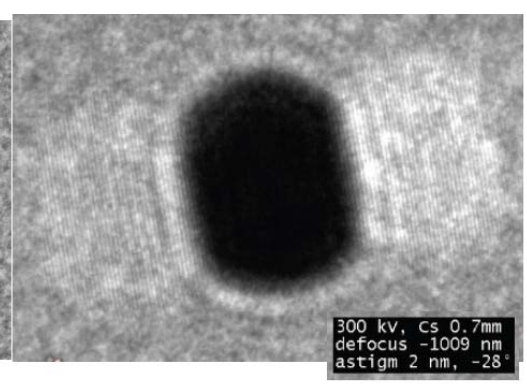
What do you notice ?

Can you figure out the underlying explanation?

"delocalisation"

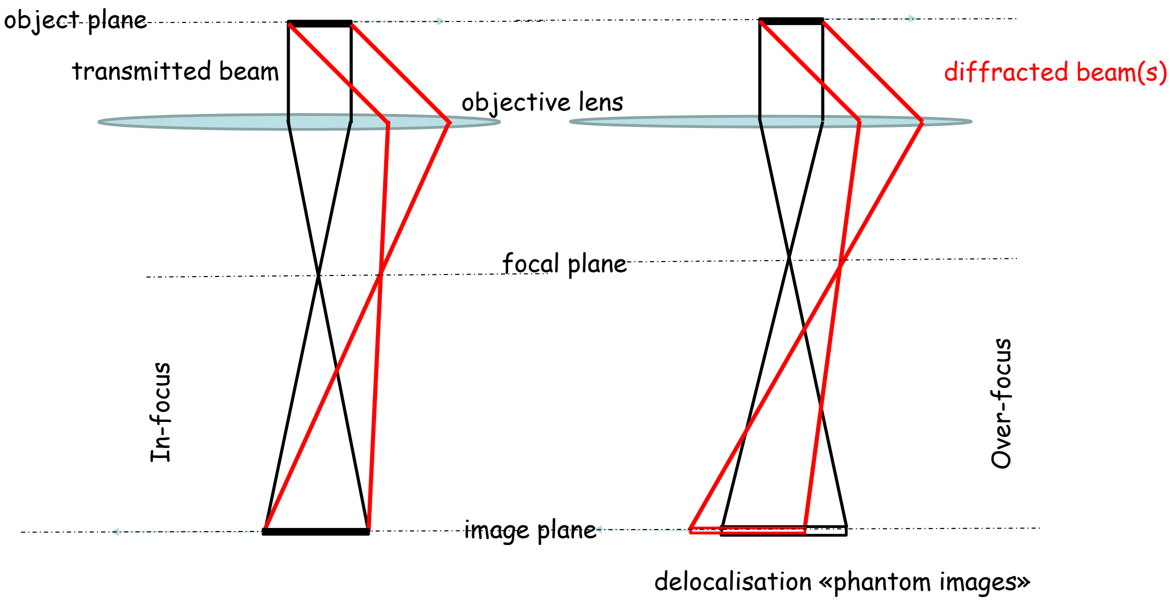




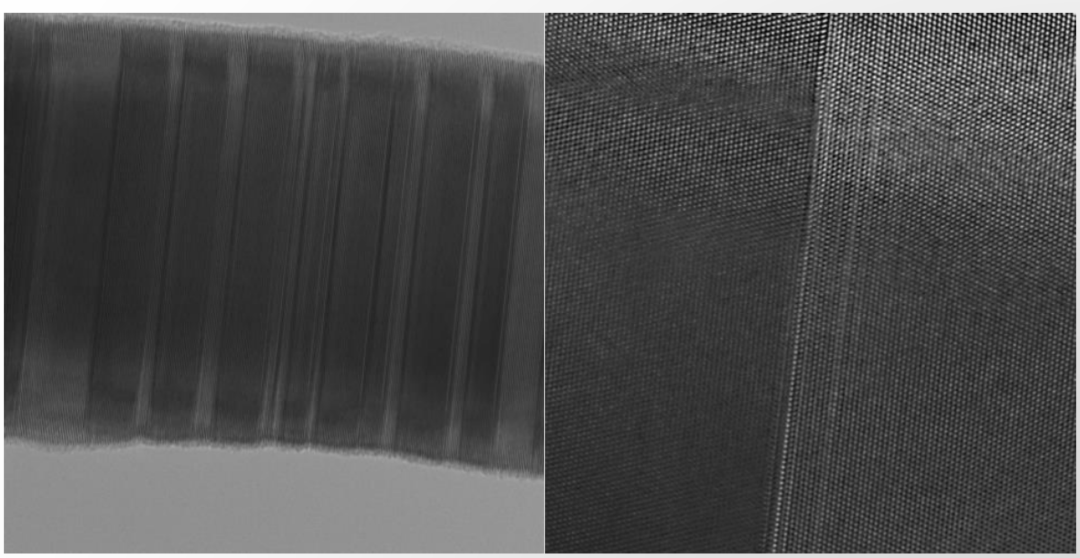


Au nanoparticle on amorphous carbon. Various defocalisation

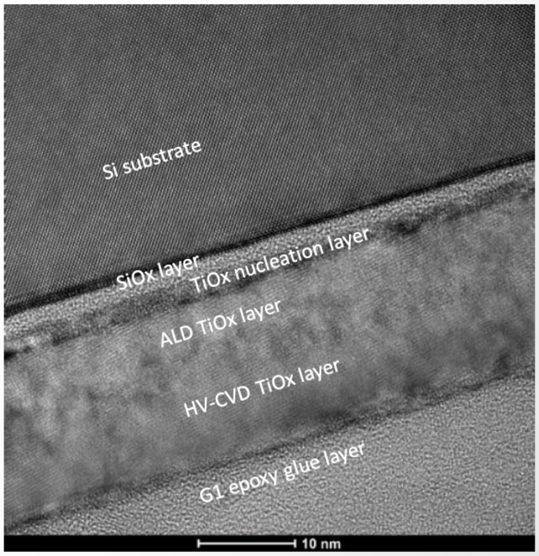
Effect of defocus <-> «phantom images»

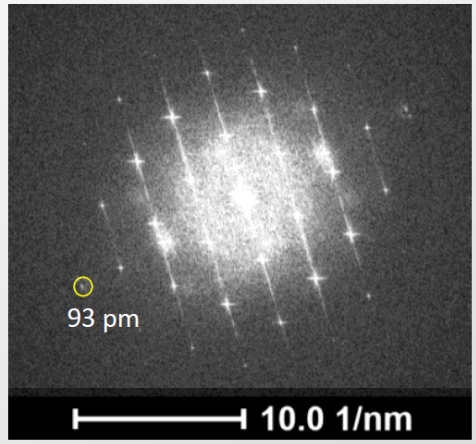


1 HRTEM examples from the Talos: imaging nanowire defects

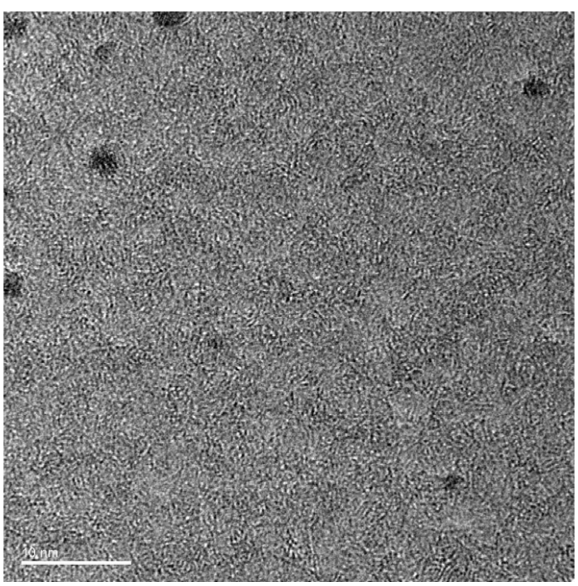


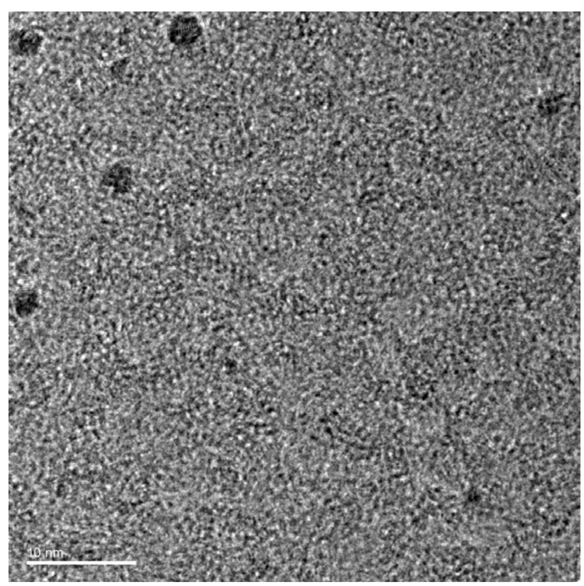
2 HRTEM examples from the Talos: imaging layer thickness and defects in thin film coatings processed with different techniques



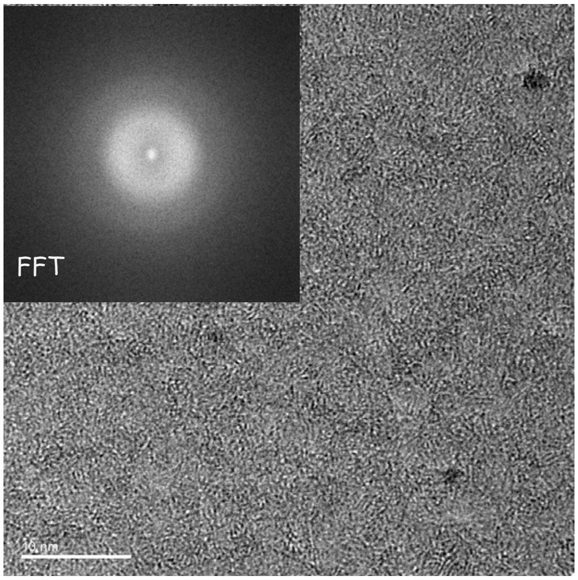


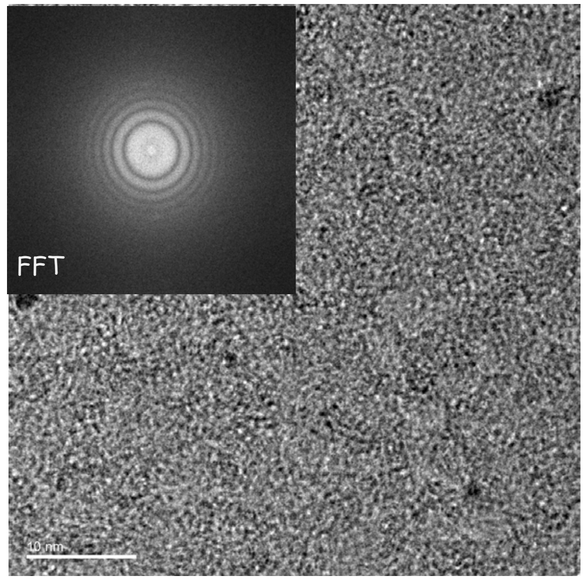
Can we see the effect of the transfer function…?



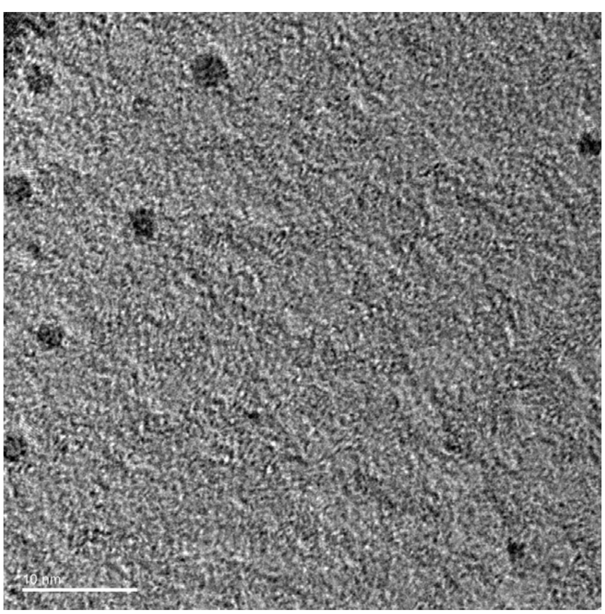


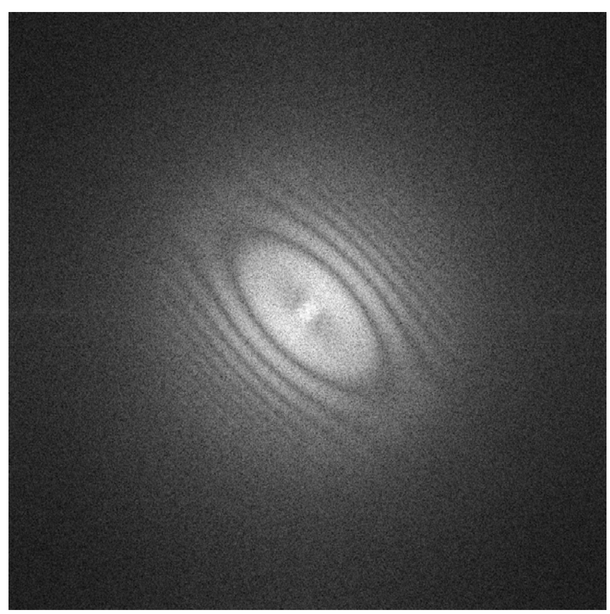
The FFT tells the «truth»



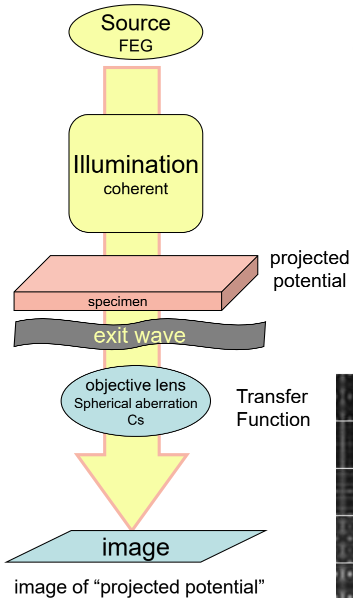


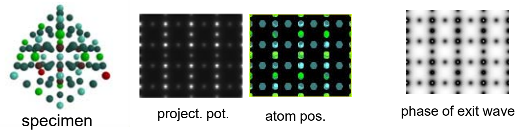
Astigmatism…

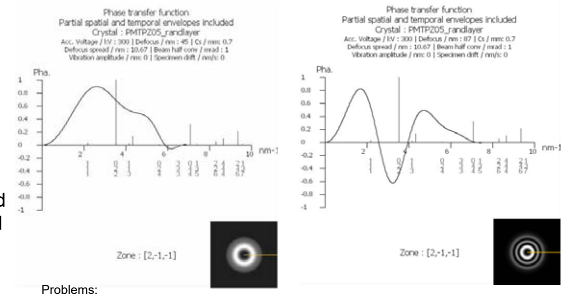




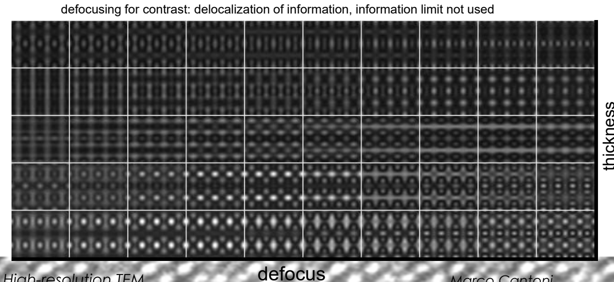
HRTEM image formation







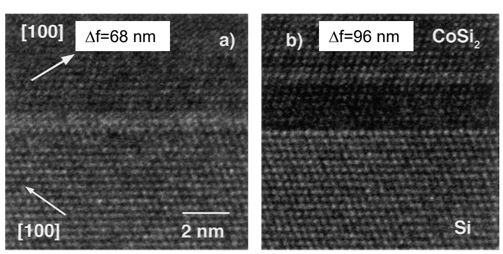
Problems:
defocusing for contrast: delocalization of information, information limit not used

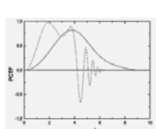


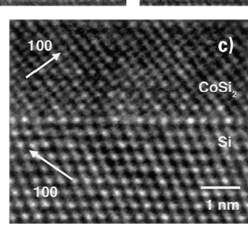
the aberration-corrected transmission electron microscope

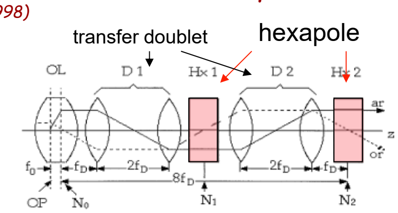
(Rose, 1990; Haider et al., 1998)

Maximilian Haider, Stephan Uhlemann,
Eugen Schwan, Harald Rose, Bernd Kabius, Knut Urban
NATURE, VOL 392, 1998

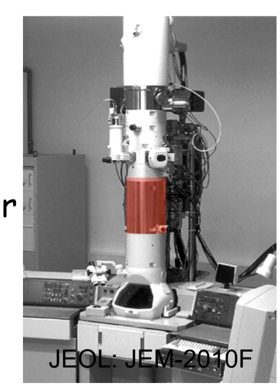








Cs-corrector

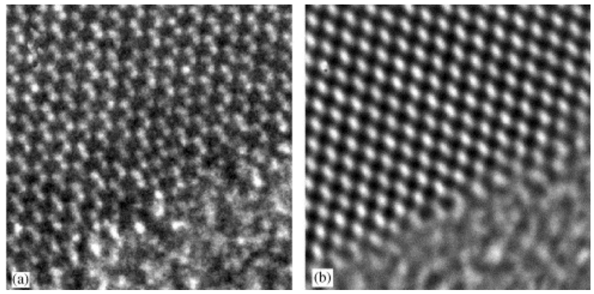


Sharp interfaces

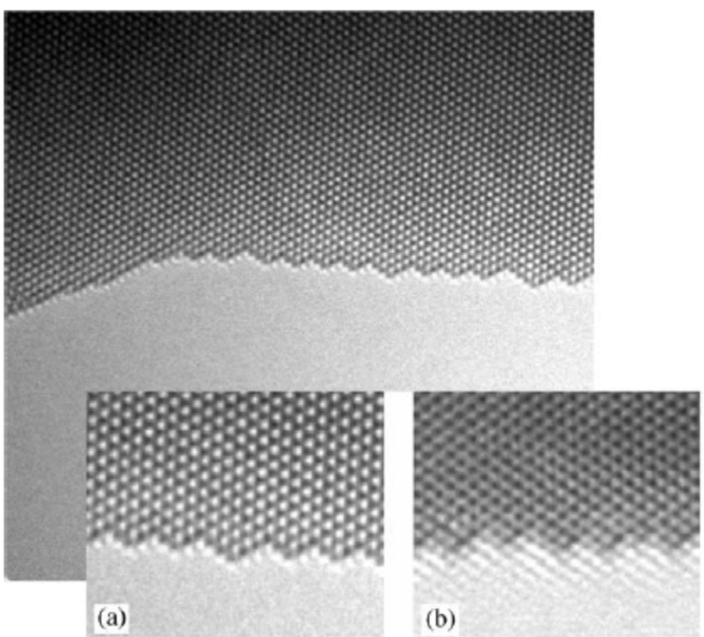
Fig. 3. TEM image of a cross section of a MOSFET transistor showing the amorphous gate oxide layer between crystalline silicon and polycrystalline silicon, recorded with monochromator on and Cs corrector on. The image was taken with 0.1 nA beam current on the CCD, 1 s exposure time, and 2 mrad half convergence angle.

No delocalisation at interfaces anymore

Cs corrector off Cs corrector on



Gold crystal



Cs corrector on (a), off (b)