Transmission Electron Microscopy

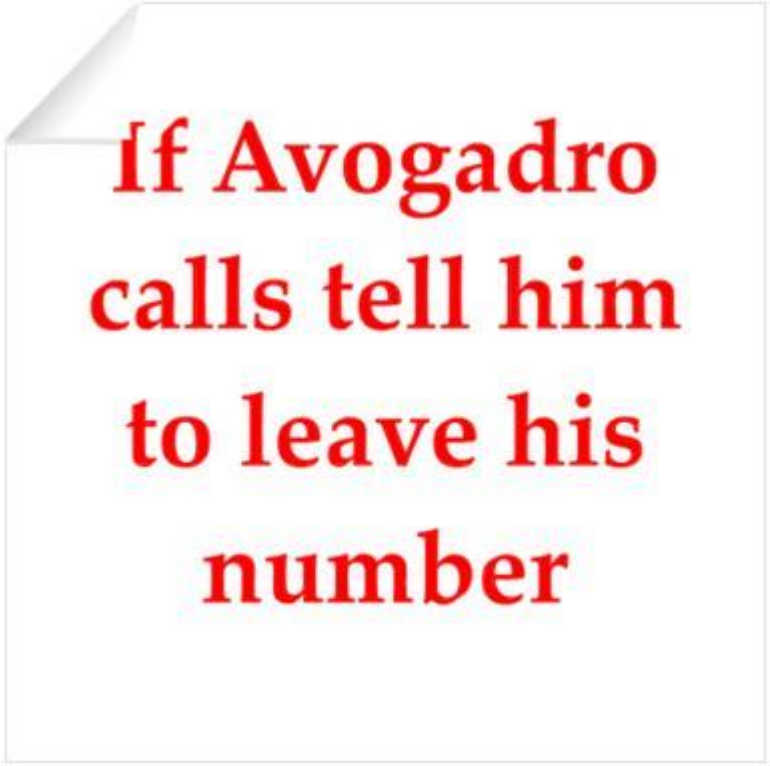
-Image Formation and Simulation-

LECTURE SERIES

HETEROGENEOUS CATALYSIS

Berlin, Dec. 5th 2014

Thomas Lunkenbein, FHI-AC
lunkenbein@fhi-berlin.mpg.de


If Avogadro
calls tell him
to leave his
number

Computing in Electron Microscopy

Image simulation	- Interpreting the image - Easy change of instrumental parameters (e.g. high voltage, focus...) - Two methods: Bloch wave eigenstates or multi-slice methods
Image processing	-Improve interpretability -Recover additional information (image restoration deconvolve transfer function of the instrument from a single image vs. image reconstruction combination of several images into one image)
Instrument design	Broad research field
On-line control	Record the data and to control the instrument
Data archiving	Digital storage vs. Photographs (degrading time)

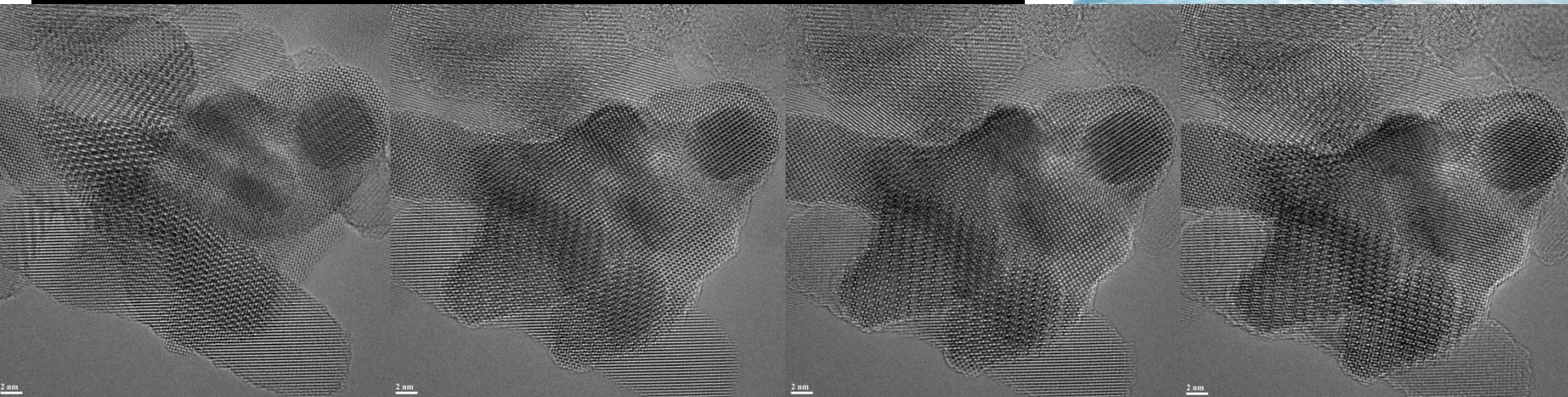
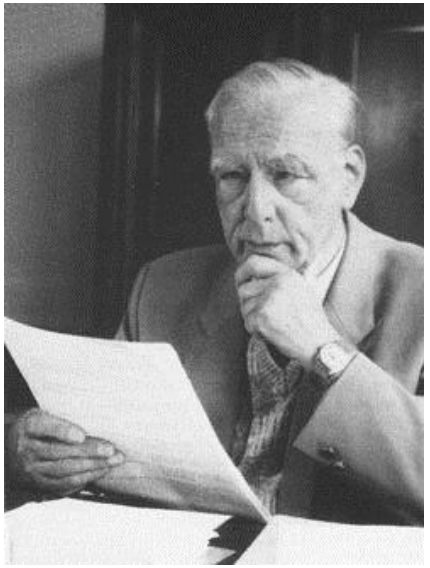


Table 1.1 Some symbols and their descriptions

Symbol	Description
a, b, c	Unit cell size of the specimen in x,y,z directions
a_0	Bohr radius (0.529 Ang.)
c	Speed of light
e	Charge on the electron
m_0	Rest mass of the electron
m	Total mass of the electron
V	Accelerating voltage
h	Planck's constant ($\hbar = h/(2\pi)$)
λ	Electron wavelength
χ	Phase error due to aberration of a focused electron wave
α	Electron scattering half angle
β	Condenser illumination half angle
x, y	Position in the image plane
z	Position along the optic axis
k	2D spatial frequency in the Fourier transform of the image plane
$K = k(C_s\lambda^3)^{1/4}$	dimensionless spatial frequency
Δf	Defocus
$C_S = C_{S3}$	Third order spherical aberration
C_{S5}	Fifth order spherical aberration
σ	Electron interaction parameter
$\frac{\partial\sigma}{\partial\Omega}$	Partial cross section for scattering

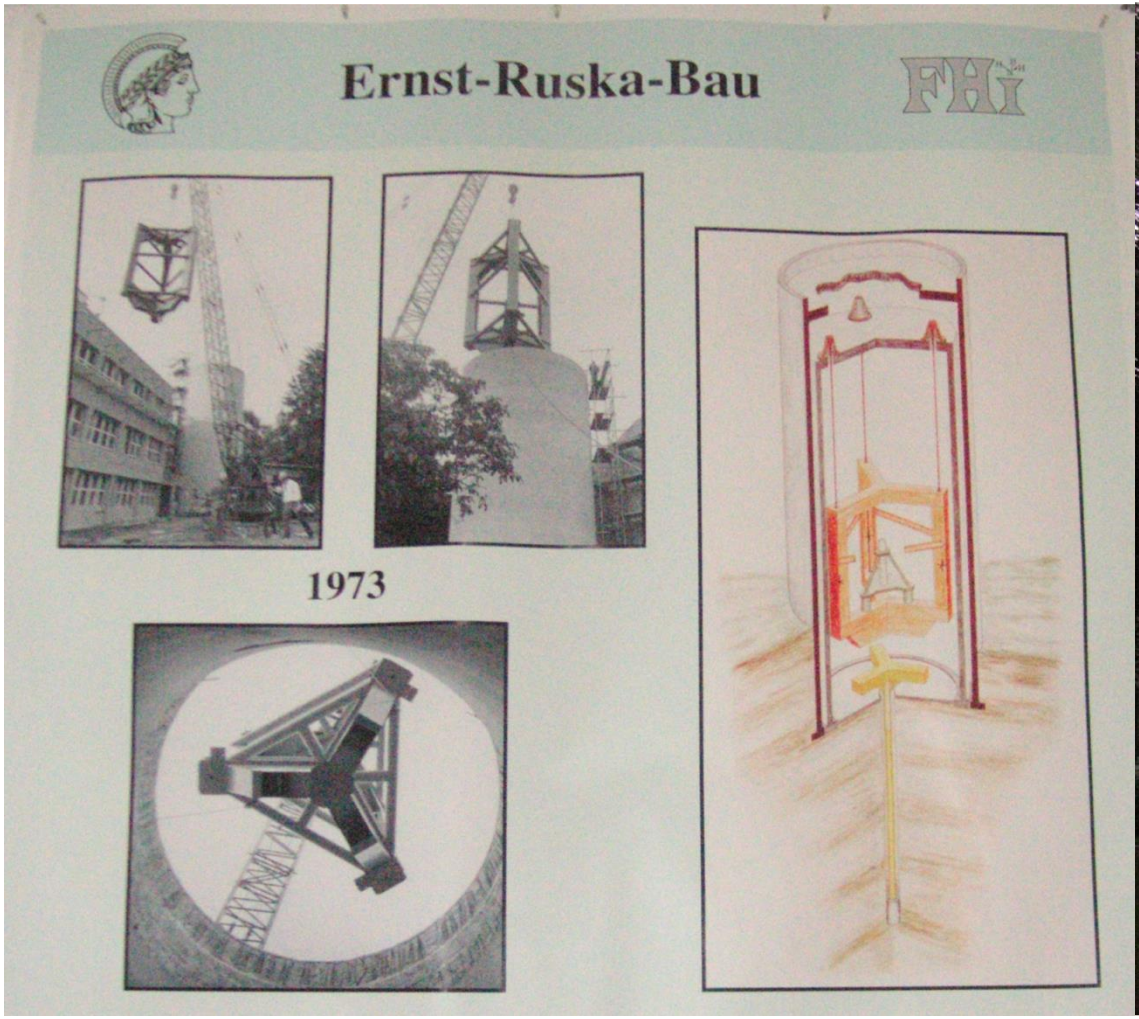
The Transmission Electron Microscope



Early 1930s: Knoll and Ruska build first TEM

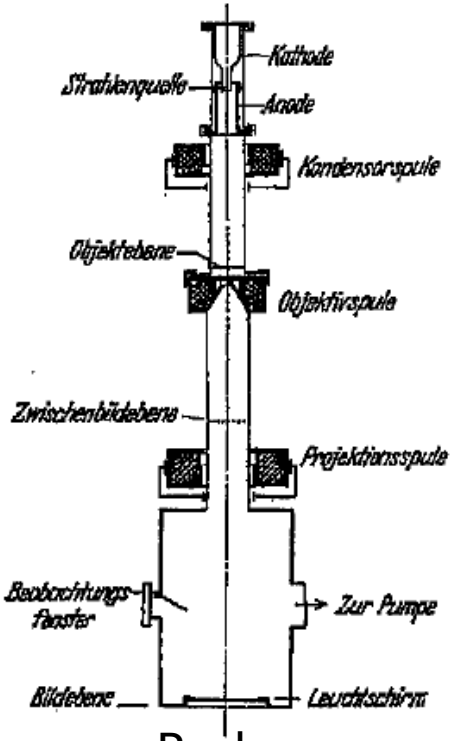
1986: Nobel Prize in physics for
Ernst Ruska (TEM),
Gerd Binnig & Heinrich Rohrer (STM)

The Transmission Electron Microscope



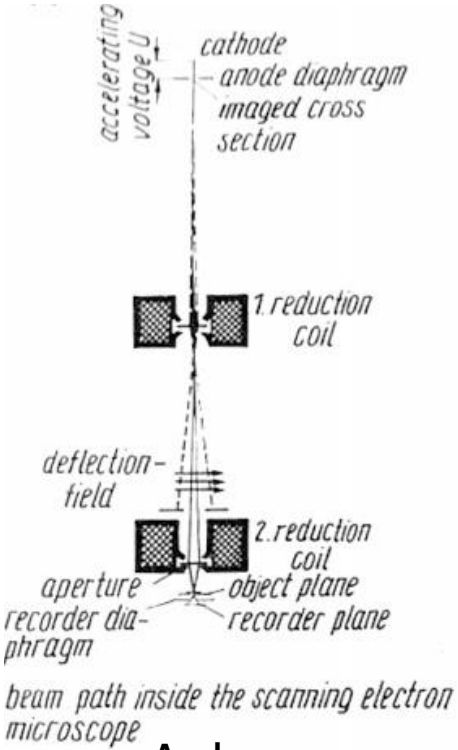
T. Lunkenbein, FHI

The Transmission Electron Microscope



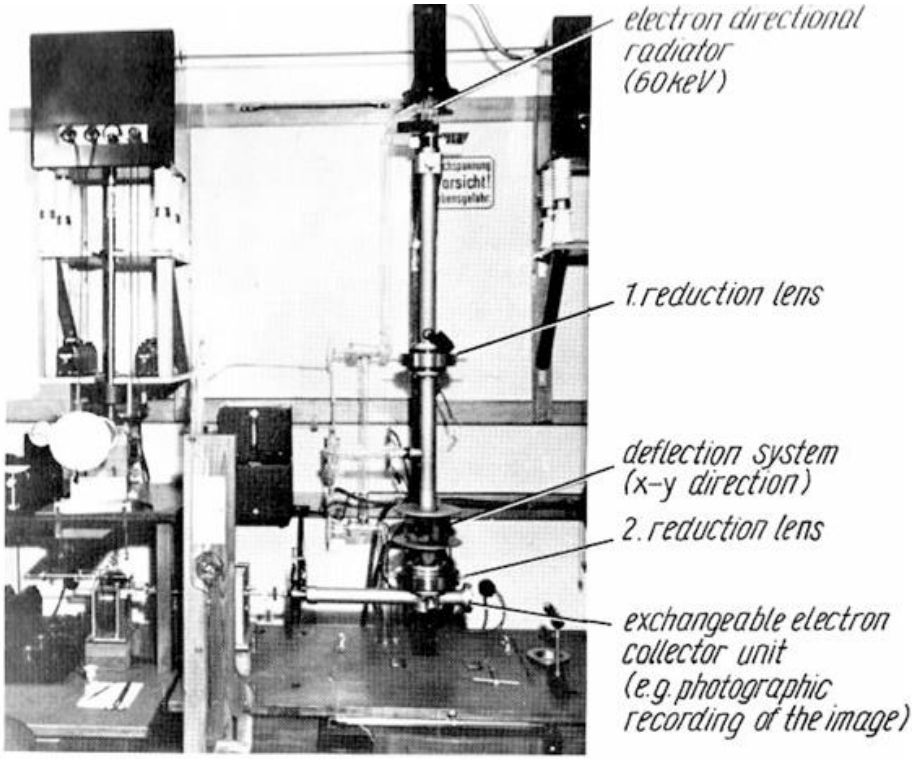
Ruska

CTEM



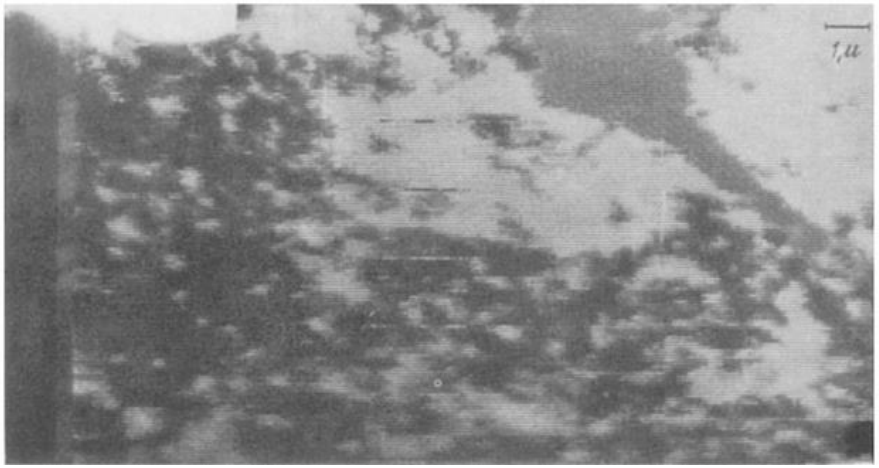
von Ardenne

STEM



Transmitted electrons will be detected

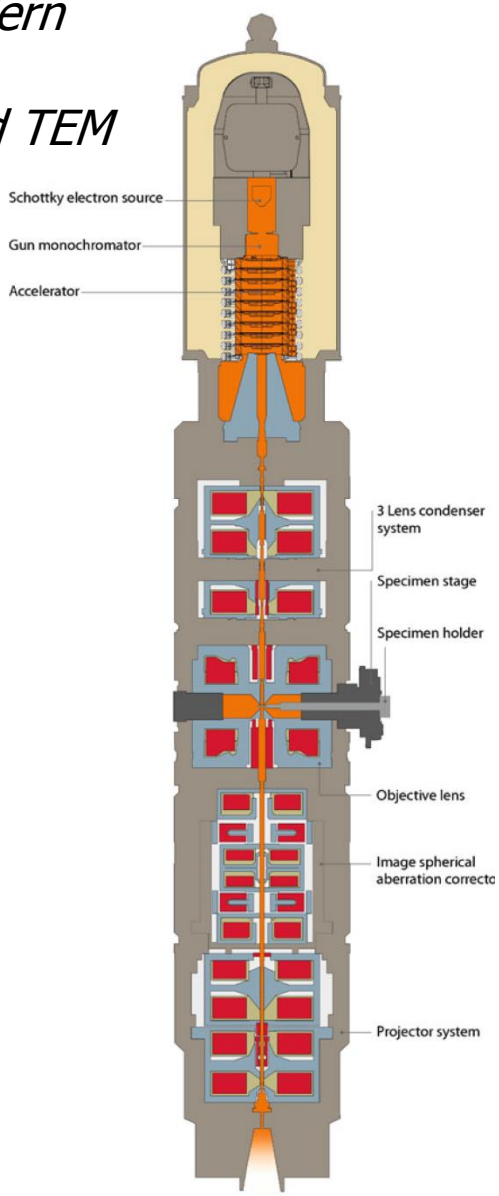
→ High energy of electrons (100-1000kV)

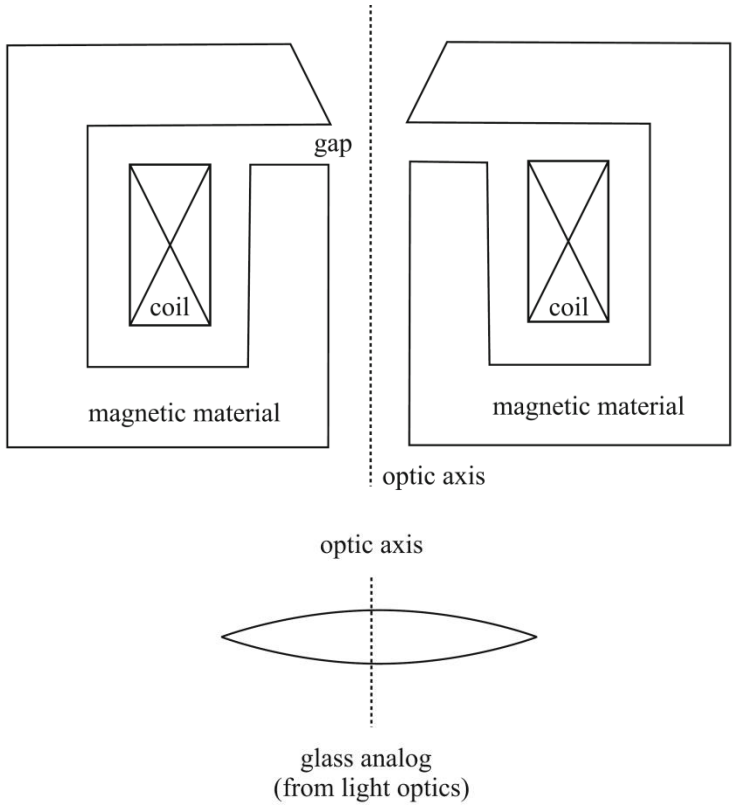


Knoll et al. *Z.Physik* **1932**, 76, 649-654.
v.Ardenne *Z.Tech.Physik* **1938**, 19, 4ß7-416.

The Transmission Electron Microscope

Scheme of a modern high resolution aberration corrected TEM

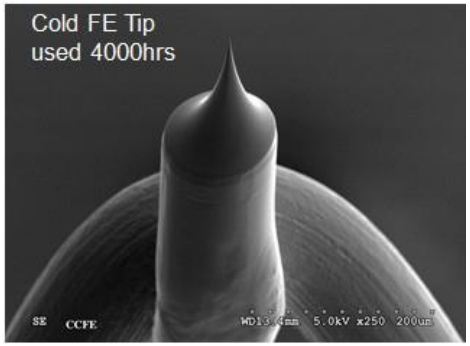


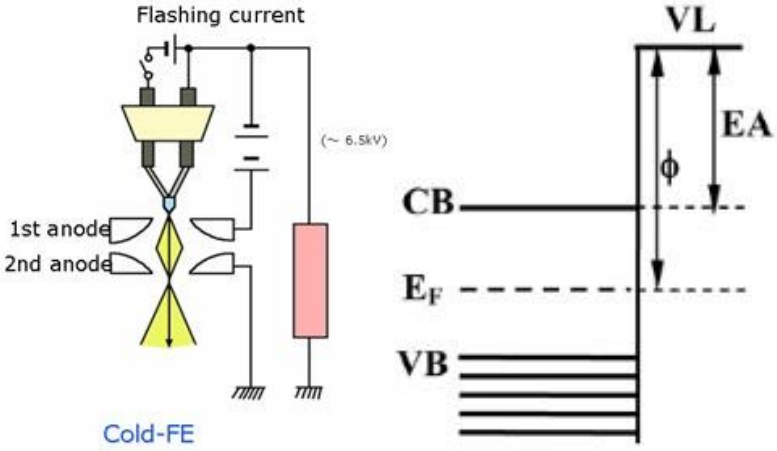


The Transmission Electron Microscope

Cold FEG vs. Schottky FEG

Effective source size: 5 nm



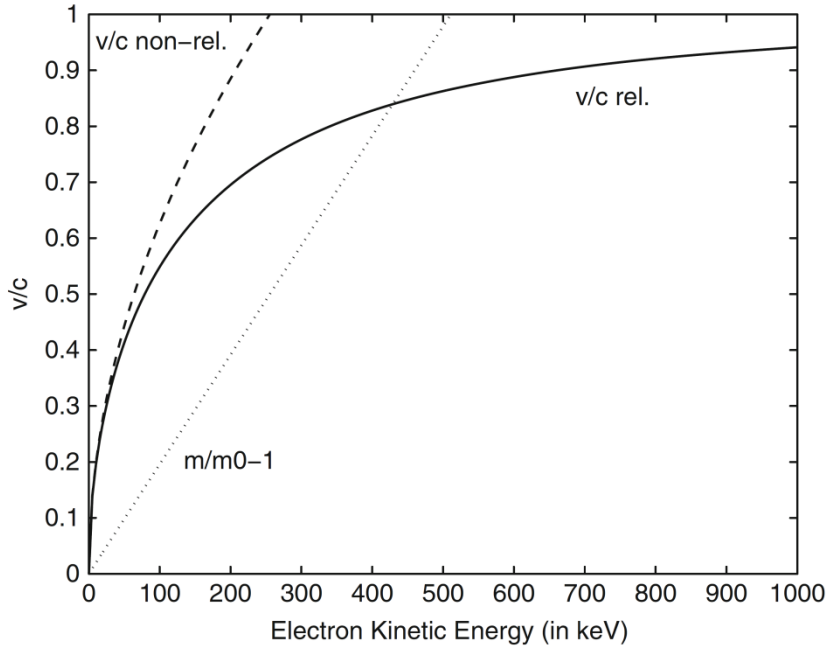


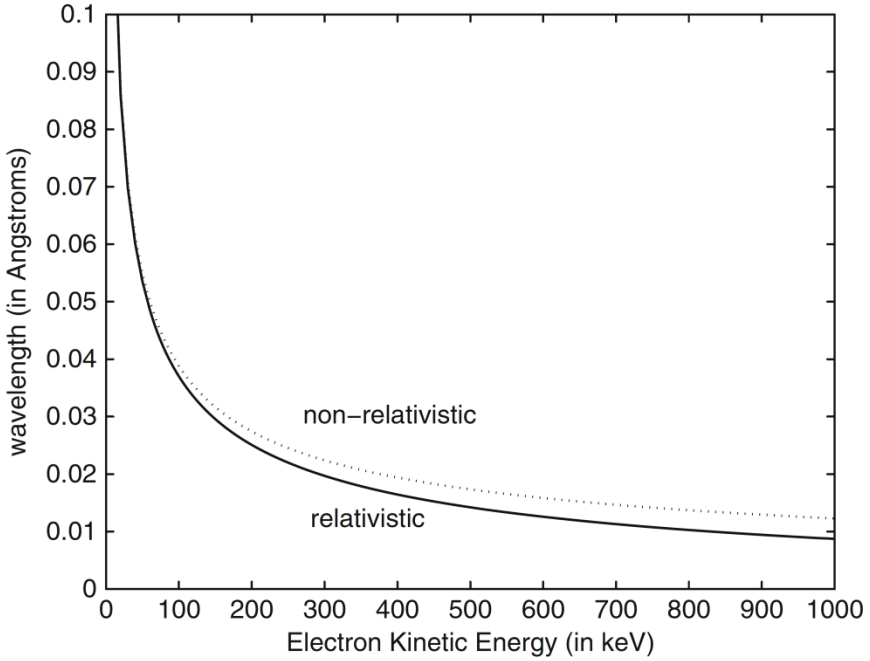
Source	Thermoionic	Thermoionic	FEG	Cold FEG
Material	W	LaB_6	W(100) + ZrO	W(310)
Work function [eV]	4.5	2.7	2.7	4.5
Tip radius [µm]	50-100	10-20	0.5-1	<0.1
Temperature [K]	2800	1900	1800	300
Normalized Brightness [$Acm^{-2}sr^{-1}$]	10^4	10^5	10^7 /10^8	$2*10^7$ /10^9
Energy spread at gun exit [eV]	1.5-2.5	1.3-2.5	0.4-0.7 /0.9	0.3-0.7 /0.22
Vacuum [Torr]			10^{-8}	10^{-10}

Dehm et al. *In-situ Electron Microscopy* 2012; spectral.se; spie.org

The Transmission Electron Microscope

Relativistic Electrons



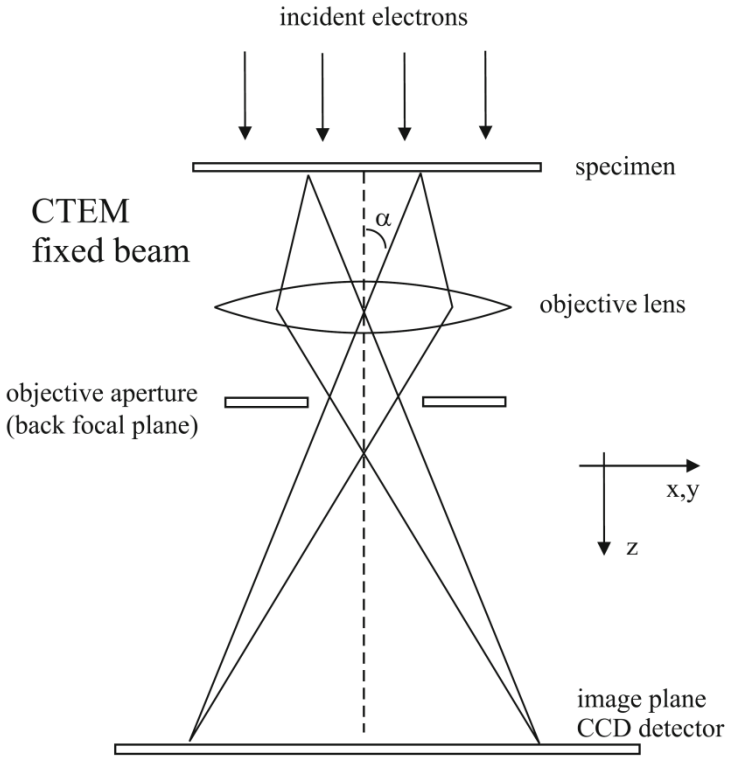


Schrödinger wave equation of quantum mechanics is not relativistically correct. The electron is relativistiv at the beam energies used in the electron microscope meaning that the relativistic Dirac equation would be the correct wave equation for relativistic electrons

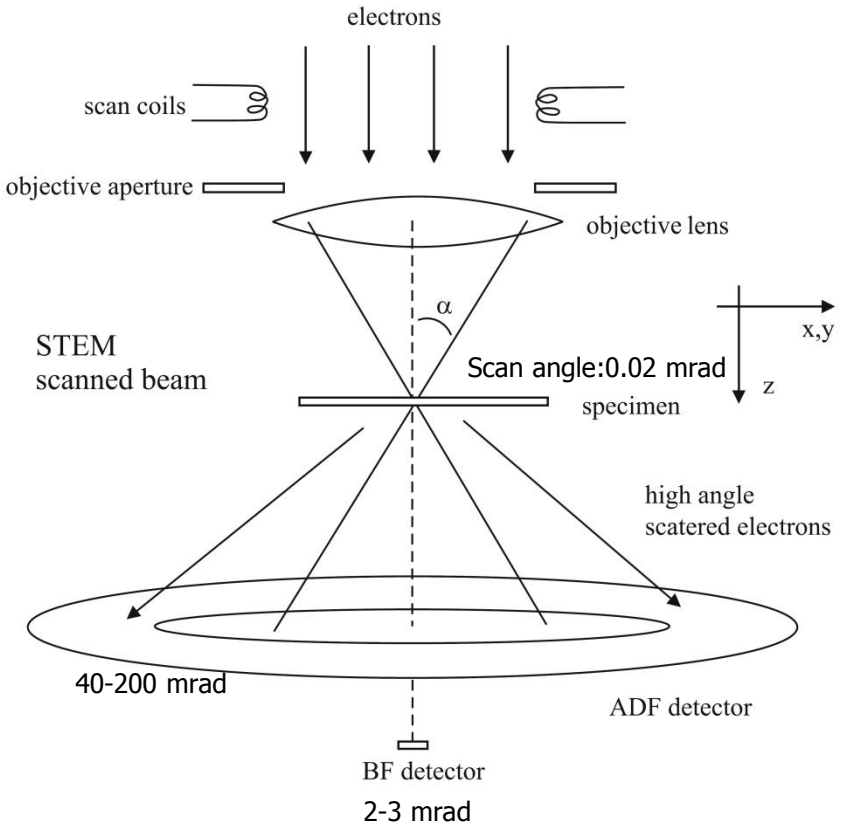
The Transmission Electron Microscope

Modelling the TEM

Sample in vacuum, illumination system (condensor) aligned



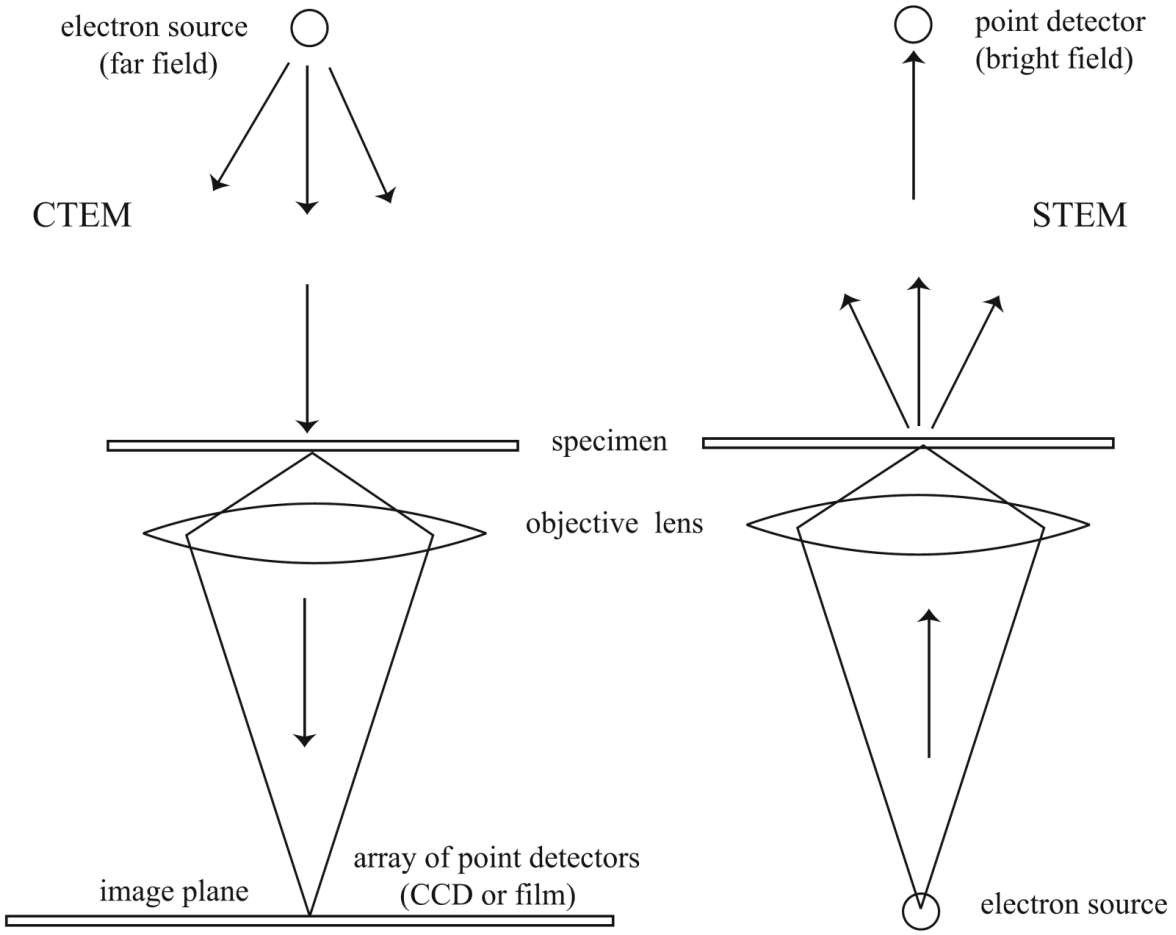
Whole image is formed in parallel



Focused probe scan across the sample and the image
Is built sequentially

The Transmission Electron Microscope

Reciprocity



Electron intensities and ray paths in the microscope remain the same if their direction is reversed and the source and detector are interchanged (electrons trajectories and elastic scattering processes have time reversal symmetry).

T. Lunkenbein, FHI

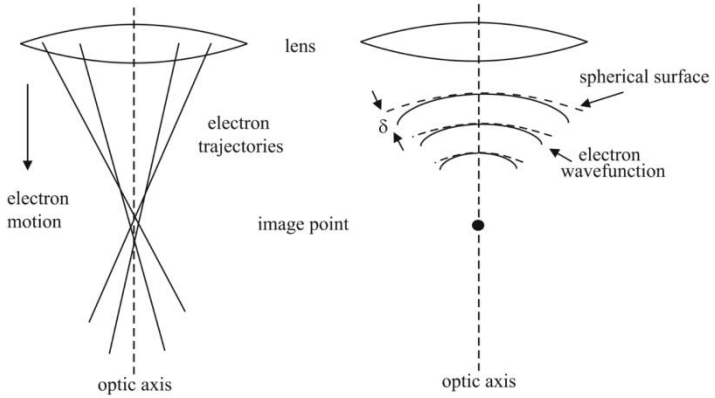
The Transmission Electron Microscope

Aberration

Most aberrations that exists for optical lenses also exists for magnetic lenses (Maxwell´equations)

Well-aligne elctron microscope higher order aberration are negligble and only third-order spherical aberration Cs has to be considered

The magnetic field further away from the axis
Is stronger than required
→electrons traveling at larger angles (α) are deflected stronger than it is required to focus them



C_s produces a position error in the electron trajectories ~3rd power of the angle and a phase error in the electron wave function ~4 th power ortional to the

phase error $\chi = (2\pi/\lambda)\delta$

$$\alpha = \sqrt{\alpha_x^2 + \alpha_y^2} \qquad \chi = \frac{2\pi}{\lambda}\delta = \frac{2\pi}{\lambda}\left(\frac{1}{2}C_1\alpha^2 + \frac{1}{4}C_3\alpha^4 + \frac{1}{6}C_5\alpha^6 + \cdots\right) \qquad \Delta f = -C_1$$

Scherzer Theorem: A static, rotationally symmetric magnetic field with no sources on the axis will always produce a spherical aberration greater than zero because the expression for Cs can be written as the sum of quadratic terms.

$$\chi(\alpha) = \frac{2\pi}{\lambda}\left(\frac{1}{4}C_s\alpha^4 - \frac{1}{2}\Delta f\alpha^2\right) \qquad \alpha = \lambda k$$

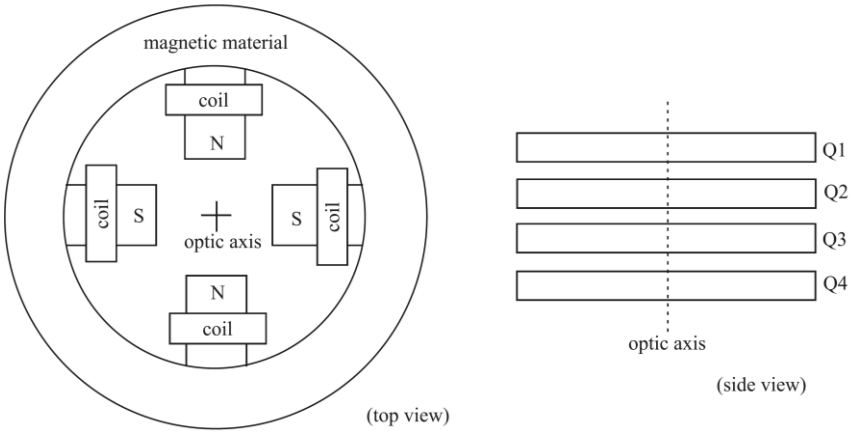
λk=α: semiangle of the ojective aperutre
Δf=-C_1: defocus
C_3=C_s: spherical aberration (3rd order)
λ= wavelength
δ: deviation

The Transmission Electron Microscope

Aberration correction

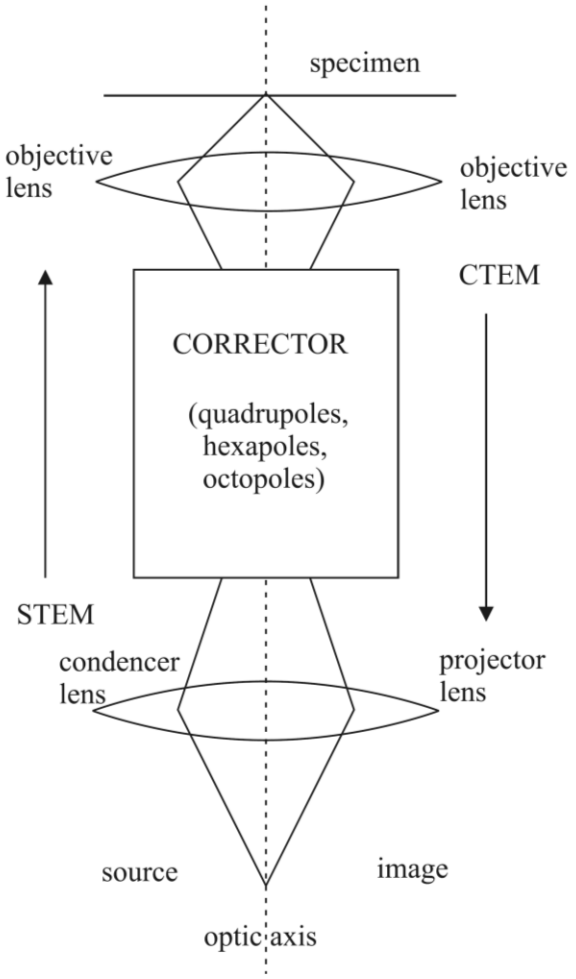
Rotational lenses have always positive aberrations

Correction: non-rotationally symmetric lenses are used
To produce negative aberrations to balance positive aberrations



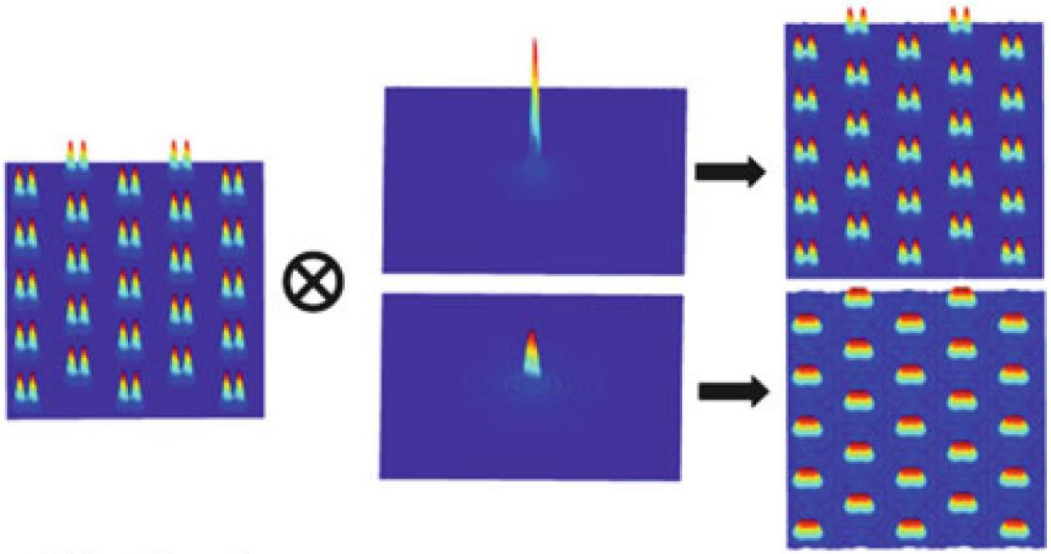
converge and diverege the beam
→ Negative aberrations

Aberration corrected TEM



Linear Image Appoximations

- Approximation to calculate TEM and STEM images using linear image models.



f(x)	h(x)	g(x)
Ideal image of the object	Representation of an image of an isolated point in the specimen *(instrument related)*	Image intensity

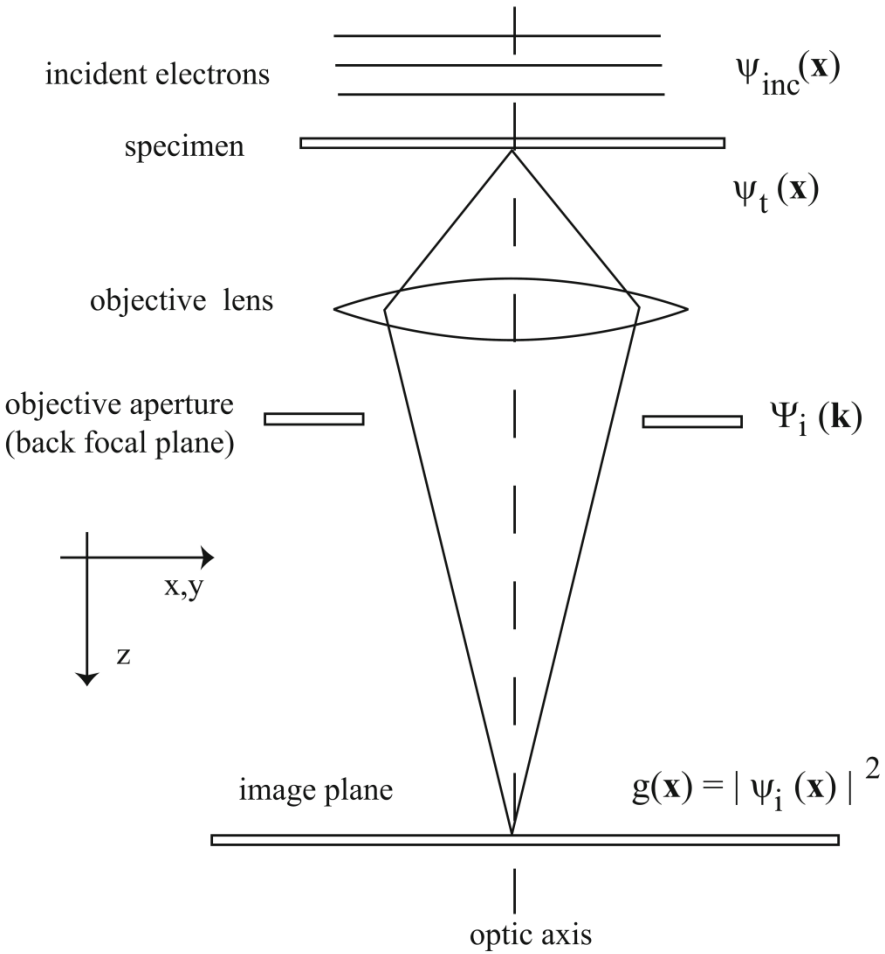
$$g(x,y) = f(x,y) \otimes h(x,y) \qquad G(\mathbf{k}) = F(\mathbf{k})H(\mathbf{k})$$

Vogt et al. – *Modelling Nanoscale Imaging in Electron Microscopy* 2012.

Linear Image Appoximations

Weak Phase Object in BF-TEM

very thin sample + only light atoms



$$\psi_t(\mathbf{x}) \sim t(\mathbf{x}) \sim \exp[i\sigma_e v_z(\mathbf{x})] \sim 1 + i\sigma_e v_z(\mathbf{x}) + \cdots$$

Fast electrons pass through a thin sample.

Electrons deviate slightly in their phase

Effect can be modeled by a transfer function (t(x))

$$\psi_t(\mathbf{x}) = t(\mathbf{x})\psi_{inc}(\mathbf{x})$$

Aberrations in the objective lens shift the phase of each frequency component

Objective lense forms an reciprocal image in the back Focal plane

$$\Psi_t(\mathbf{k}) = \mathrm{FT}[\psi_t(\mathbf{x})]$$
$$\Psi_i(\mathbf{k}) = \Psi_t(\mathbf{k})\exp[-i\chi(\mathbf{k})] = \Psi_t(\mathbf{k})H_0(\mathbf{k})$$

Objective lens images this wave function
→inverse FT

Recorded image is the intensity of the image Wave function

$$g(\mathbf{x}) = |\psi_i(\mathbf{x})|^2 = |\psi_t(\mathbf{x}) \otimes h_0(\mathbf{x})|^2$$

- Specimen shall produce a phase shift in the electron wave function
- Weak specimen: exponential phase factor can be expanded in a power series
-Only low order terms are important

Linear Image Appoximations

Weak Phase Object in BF-TEM

$$G(\mathbf{k}) = \mathrm{FT}[g(\mathbf{x})] = \delta(\mathbf{k}) + 2\sigma_e V_z(\mathbf{k}) H_{\mathrm{WP}}(\mathbf{k})$$

$$H_{\mathrm{WP}}(\mathbf{k}) = \mathrm{FT}\left[h_{\mathrm{WP}}(\mathbf{x})\right]$$

$$= \frac{i}{2}\{\exp[-i\chi(\mathbf{k})] - \exp[i\chi(\mathbf{k})]\}$$

$$= \sin\chi(\mathbf{k}).$$

Problem!!!

Some spacinges will be transmitted as white ($H_{WP}(k)>0$); at the same time other spacing are transmitted black ($H_{WP}(k)<0$)

-but: minimum of $H_{WP}(k)$ remains flat for significant region

If focus is adjusted so that the sin function is close to its minimum or maximum

→$H_{WP}(k)$ has a region of uniformly transferred information

Solution!!!

→

$$0.7 \leq |\sin\chi(k)| \leq 1.0$$

$$\chi(k) = -\left[\frac{2n_D - 1}{2}\right]\pi \pm \frac{\pi}{4}$$

$$n_D = 1, 2, 3, \ldots$$

$$\chi(K) = \pi(0.5(\sqrt{D})^4 - D(\sqrt{D})^2)$$

$$D = \sqrt{2n_D - 0.5}$$

$$\Delta f = \sqrt{(2n_D - 0.5)C_s\lambda}$$

$$n_D = 1, 2, 3, \ldots$$

$$n_D = 1$$

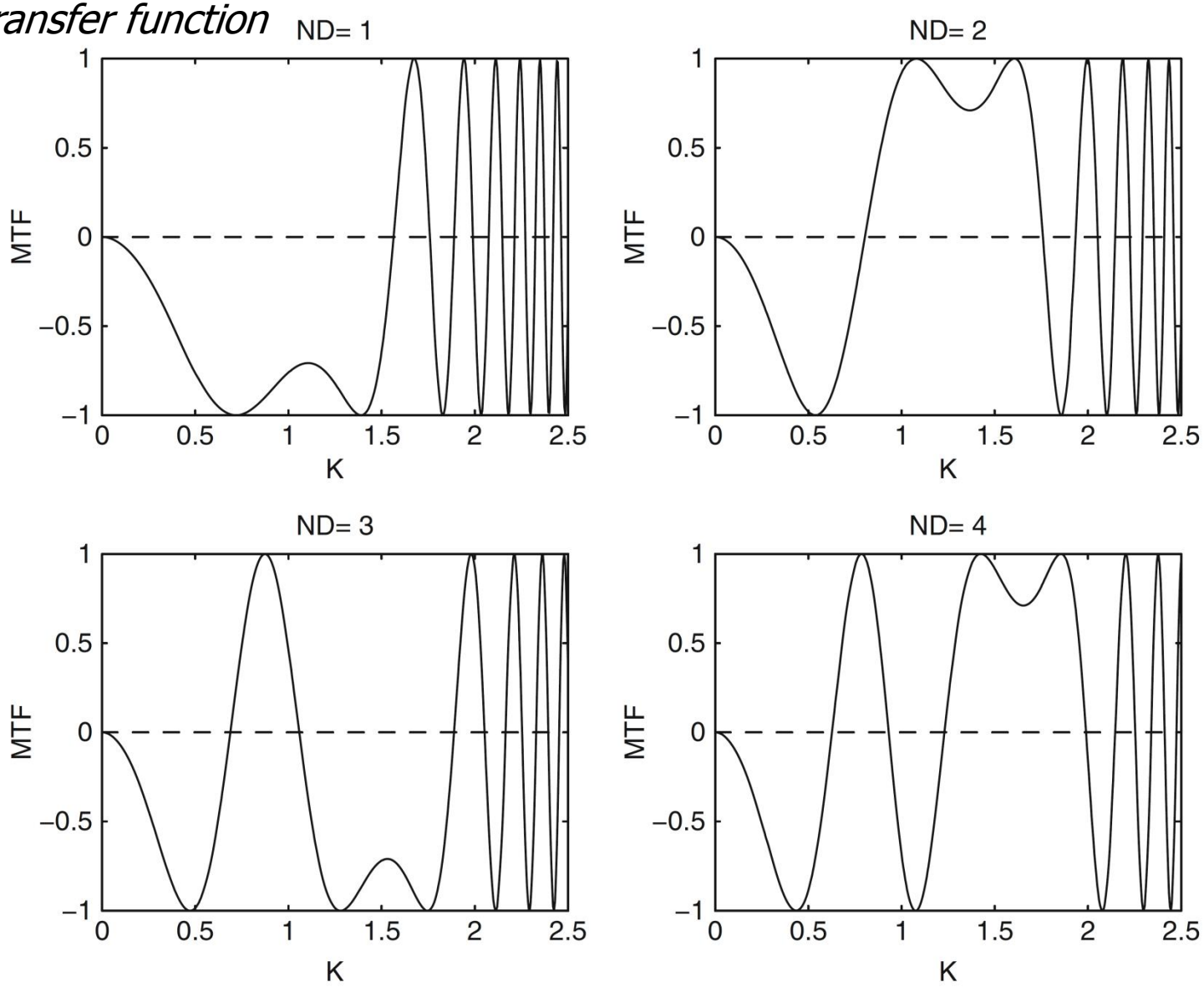
Scherzer focus

σ= interaction parameter
χ(k)= aberration function
n_D: integer numbers
C_s: spherical aberration
D: dimensionless defocus
λ=wavelength
Δf: defocus

T. Lunkenbein, FHI

Linear Image Appoximations

Contrast transfer function



Linear Image Appoximations

Scherzer Condition

Better to limit the range of spatial frequencies

→ Transfer function has same sign over the Allowed range

→place objective aperture in the back focal plane Of the objective lens

→$r_{aperture}$ corresponds to the spatial frequency

All rays within a maximum of the optical axis are Allowed to pass

→ Objective aperture limits the maximum Spatial frequency in the image

→CTF has same sign over the range

$$\alpha_{max} = \lambda k_{max} = \left(\frac{6\lambda}{C_s}\right)^{1/4}$$

+

$$D = \sqrt{1.5}$$

||

Scherzer condition

Scherzer aperture

Corresponds to the first zero crossing of the transfer function

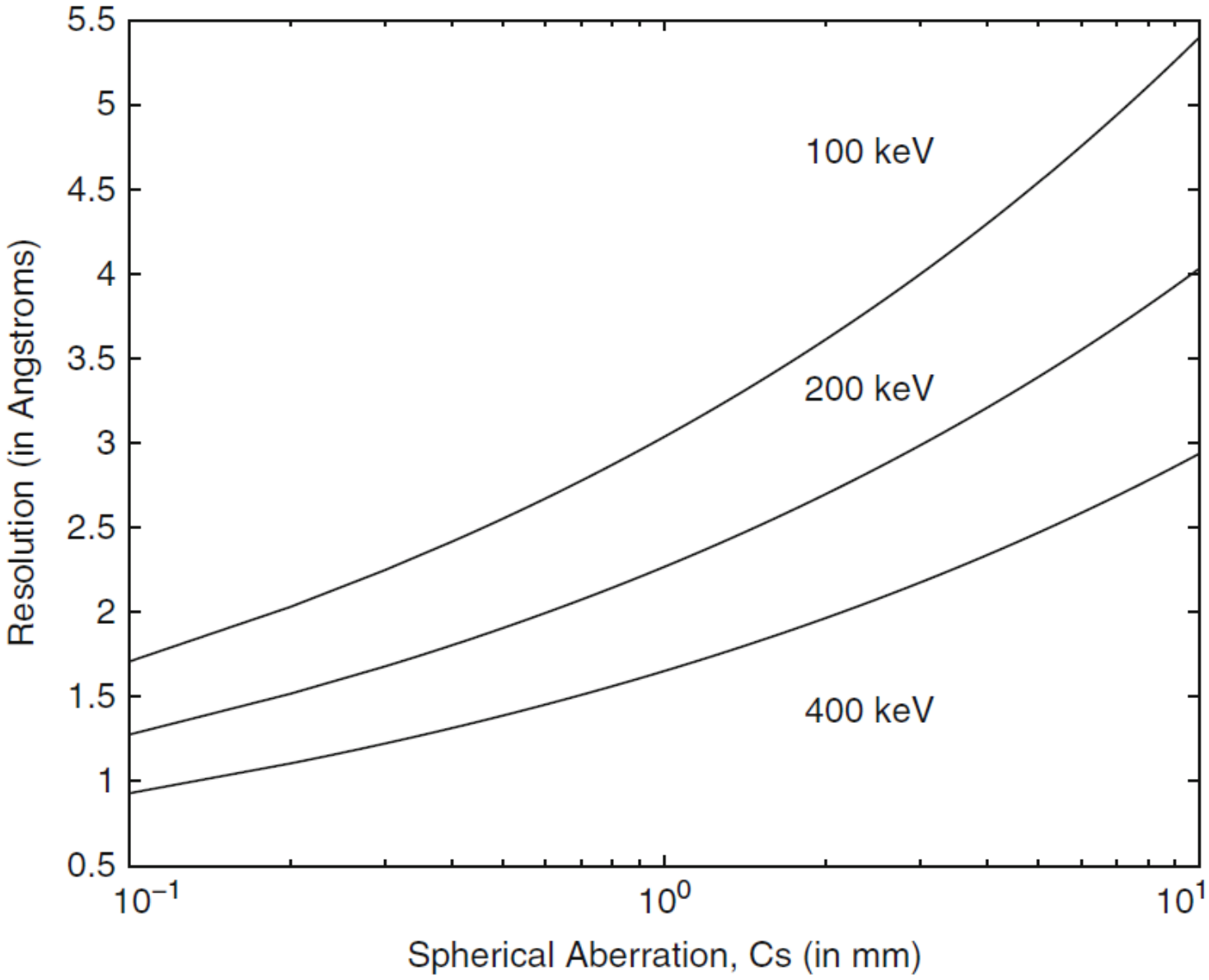
Scherzer focus

Resolution at Scherzer condition:

$$d_s > \left(\frac{C_s\lambda^3}{6}\right)^{1/4} = 0.64(C_s\lambda^3)^{1/4} = 1/k_{max}$$

λ: wavelength
C_s: spherical aberrations
k_{max}: maximum spatial frequency

Linear Image Appoximations



Linear Image Appoximations

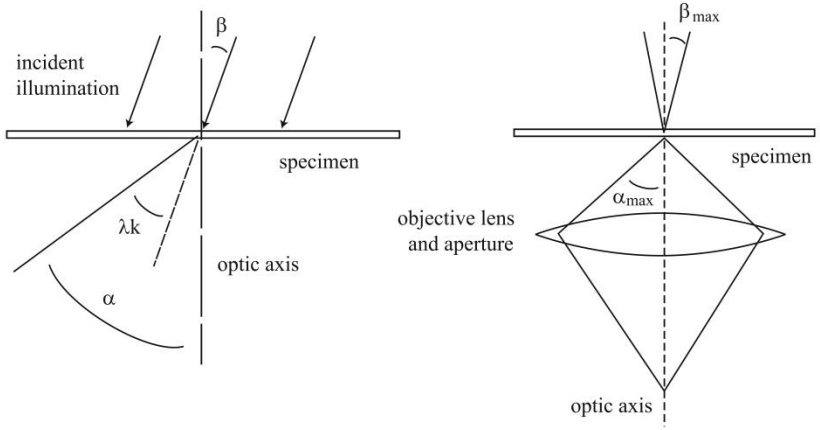
Partial Coherence

Imaging with none ideal illumination

Condenser delivers a small cone of
Illumination on the sample;

Each illumination angle will be incoherent
With other angles

→adding intensities and amplitudes



Transmitted wave function function of the specimen:

$$\psi_t(\mathbf{x}) = t(\mathbf{x})\exp(2\pi i\mathbf{k}_\beta \cdot \mathbf{x})$$

Image intensity:

Energy fluctuations contribute to the defocus fluctuations

$$g(\mathbf{x}) = \int |\psi_i(\mathbf{x})|^2 p(\mathbf{k}_\beta) p(\delta_f) \mathrm{d}\delta_f \mathrm{d}^2 k_\beta$$

$$= \int \left| \left[t(\mathbf{x})\exp(2\pi i\mathbf{k}_\beta \cdot \mathbf{x}) \right] \otimes h_0(\mathbf{x}, \Delta f + \delta_f) \right|^2 p(\mathbf{k}_\beta) p(\delta_f) \mathrm{d}\delta_f \mathrm{d}^2 k_\beta$$

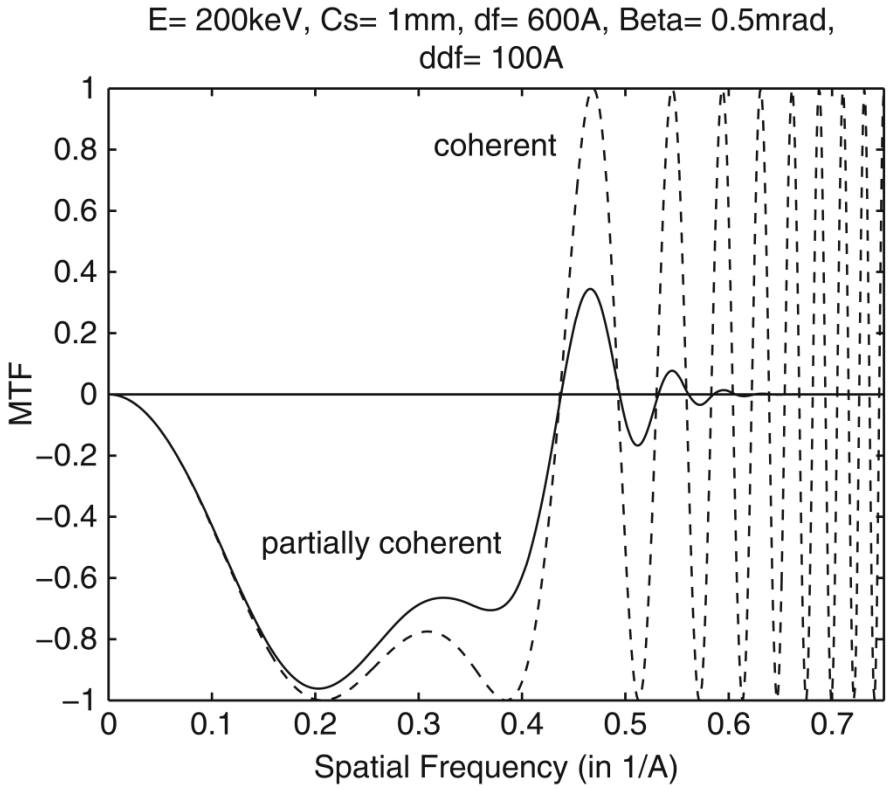
Δf: defocus
$p(\mathbf{k}_\beta)$: distribution of illumination angles
$p(\delta_f)$: distribution of the fluctuation of the defocus
δ_f: fluctuation in defocus
$\beta = \lambda \mathbf{k}_\beta$: angle of incident illumination (with Respect to the optical axis

Linear Image Appoximations

Transfer function of the objective lens:

$$H_{\mathrm{WP}}(k) = \sin\left[\frac{\pi\lambda k^2}{1+\varepsilon k^2}\left(0.5C_s(1-\varepsilon k^2)\lambda^2 k^2 - \Delta f\right)\right]$$

$$\times \frac{1}{\sqrt{1+\varepsilon k^2}} \exp\left[-\frac{[\pi\lambda k_s k(C_s\lambda^2 k^2 - \Delta f)]^2 + 0.25(\pi\lambda\Delta_0 k^2)^2}{1+\varepsilon k^2}\right]$$



$\varepsilon = \pi\lambda k_s \Delta_0$
$k_s = K_s(C_s\lambda^3)^{-1/4}$
$\Delta_0 = D_s(C_s\lambda)^{1/2}$: rms value of all fluctuations
λ: wavelength
D_s: Spread in defocus values
K_s: Spread in illumination angles
Δf: defocus
$\beta = \lambda k_s$: condenser semiangle
C_s: spherical aberrations

Linear Image Appoximations

$\varepsilon=\pi\lambda k_s\Delta_0$
$k_s=K_s(C_s\lambda^3)^{-1/4}$
$\Delta_0=D_s(C_s\,\lambda)^{1/2}$: rms value of all fluctuations
λ: wavelength
D_s: Spread in defocus values
K_s: Spread in illumination angles
Δf: defocus
$\beta=\lambda k_s$: condenser semiangle
C_s: spherical aberrations

Higher aberrations

$$H_{\mathrm{WP}}(k)=\frac{1}{\sqrt{1+\varepsilon k^2}}$$

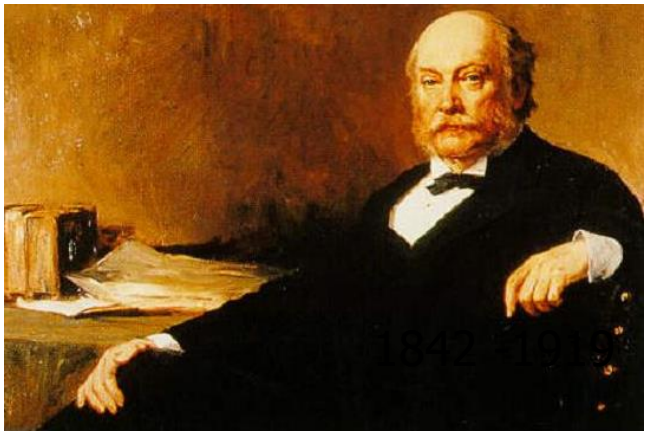
$$\times\sin\left[\frac{\pi\lambda k^2}{1+\varepsilon k^2}\left(\frac{1}{3}C_{S5}(1-2\varepsilon k^2)\lambda^4k^4+0.5C_{S3}(1-\varepsilon k^2)\lambda^2k^2-\Delta f\right)\right]$$

$$\times\exp\left[-\frac{[\pi\lambda k_s k(C_{S5}\lambda^4k^4+C_{S3}\lambda^2k^2-\Delta f)]^2+0.25(\pi\lambda\Delta_0k^2)^2}{1+\varepsilon k^2}\right].$$

Detector Influence

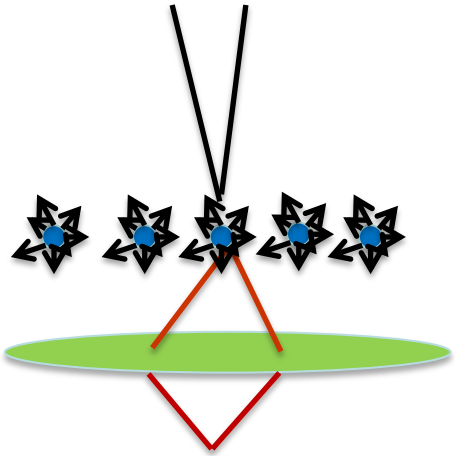
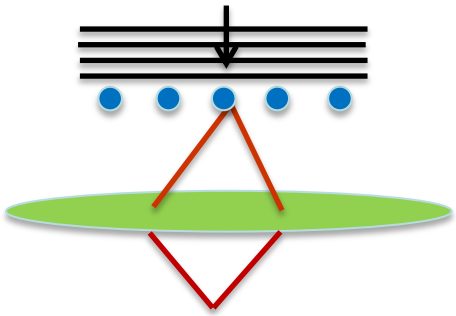
$$g(\mathbf{x})=\left|\psi_t(\mathbf{x})\otimes h_0(\mathbf{x})\right|^2\otimes h_{\mathrm{DET}}(\mathbf{x})$$

Incoherent vs. Coherent Imaging



Lord Rayleigh
1842-1919

„The function of the condenser in microscopic practice is to cause the obeject to behave, at any rate in some degree, as if it were self-luminous, and thus to obviate the sharply-marked interference bands which arise when permanent and definite phase relationships are permitted to exist between the radiations which issue from various points of the object."

STEM	TEM
self-luminous object	plane wave
	
No phase relationship (one atom column at one time)	Permanent phase relationship between neighbours
No interference is observable	Multi slit experiment
direct interpretation possible (Z contrast)	Interference occurs
	No direct interpretation possible (phase loss)

Incoherent Imaging gives significantly better resolution than coherent imaging

Nellsit et al. *Advances in Imaging and Electron Physics* 113, 147-203.

Linear Image Appoximations

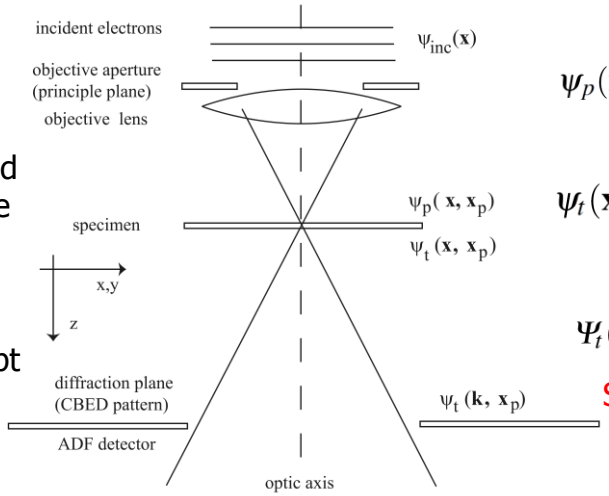
Annular Dark Field STEM

The order of optical components of the STEM is reversed from that of the TEM
i.e. objective lens before specimen

Transmitted electrons fall on detector
→form image brightness at one point

Complete image: scanning with a focused
Probe over the specimen + recording the
Transmitted intensity at each position of
the probe

The detector integrates everything except
The center region (annular detector)



$\lambda\mathbf{k}_{max}=\boldsymbol{\alpha}_{max}$: maximumg angle in the objective aperutre
$\mathbf{x}_p$: deflected probe position
$\mathbf{A}_p$: normalization constant
$\mathbf{D(k)}$: detector function

$$\psi_p(\mathbf{x},\mathbf{x}_p) = A_p \int_0^{k_{max}} \exp[-i\chi(\mathbf{k}) - 2\pi i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}_p)]d^2\mathbf{k}$$

$$\psi_t(\mathbf{x},\mathbf{x}_p) = t(\mathbf{x})\psi_p(\mathbf{x},\mathbf{x}_p)$$

$$\Psi_t(\mathbf{k},\mathbf{x}_p) = \mathrm{FT}[\psi_t(\mathbf{x},\mathbf{x}_p)] = \int \exp(2\pi i\mathbf{k}\cdot\mathbf{x})\psi_t(\mathbf{x},\mathbf{x}_p)d^2\mathbf{x}$$

STEM image signal — CBED

$$g(\mathbf{x}_p) = \int |\Psi_t(\mathbf{k},\mathbf{x}_p)|^2 D(\mathbf{k})d^2\mathbf{k}$$

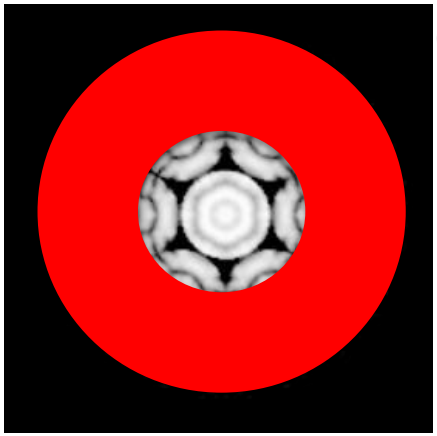
$$D(\mathbf{k}) = 1 \quad \text{for } k_{D\min} \le k \le k_{D\max}$$
$$= 0 \text{ otherwise,}$$

Incoherent image model → phase contrast negligible
+ image predominantly amplitude contrast

The probe size is limited by the aberrations of the objective lens.

Deflecting the beam to different positions changes the angles through the objetive lens
At high resolution this deflection angle is aroung 0.01 mrad.

$$\beta_{max} \ll 0.16\alpha_{max} \quad \text{coherent imaging}$$
$$\beta_{max} \gg 0.16\alpha_{max} \quad \text{incoherent imaging}$$



CBED

T. Lunkenbein, FHI

Linear Image Appoximations

Annular Dark Field STEM

→ Linear image model for incoherent scattering:

$$g(\mathbf{x}) = f(\mathbf{x}) \otimes h_{\mathrm{ADF}}(\mathbf{x})$$

Object function (probability for scattering to large angles)

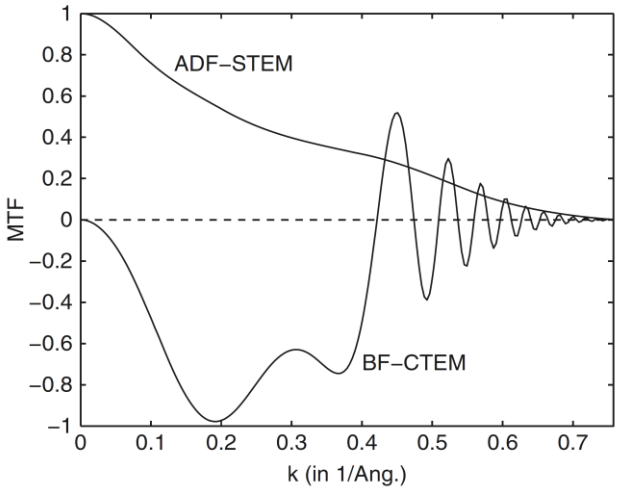
$$f(\mathbf{x}) \sim \int D(\mathbf{k}) \frac{\partial \sigma(\mathbf{x})}{\partial k_s} \mathrm{d}^2 k_s = \int_{k_{D\min}}^{k_{D\max}} \frac{\partial \sigma(\mathbf{x})}{\partial k_s} \mathrm{d}^2 k_s$$

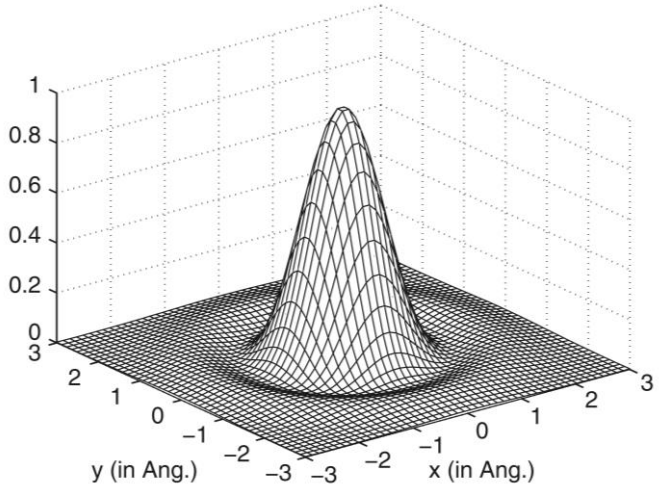
$\frac{\partial \sigma(x)}{\partial k_s}$: partial cross section for scattering to angle k_s at position x
D(k): detector function
χ(k): aberration function
A_p: Normalization constant

Point spread function (intensity distribution in the focused probe)

$$\begin{aligned} h_{\mathrm{ADF}}(\mathbf{x}) &= |\psi_p(\mathbf{x})|^2 \\ &= A_p \left| \int_0^{k_{\max}} \exp[-\mathrm{i}\chi(\mathbf{k}) - 2\pi \mathrm{i}\mathbf{k}\cdot\mathbf{x}] \mathrm{d}^2\mathbf{k} \right|^2 \end{aligned}$$

Transfer function (FT of Point spread function)





Linear Image Appoximations

Source Size

Probe: Image of the electron source (can contribute to the probe size)

Brightness of the source

$$\beta = \frac{j}{\pi\alpha^2}$$

j= current density in the probe
α= convergence half angle
β= brightness
$\mathbf{I_P}$= probe current
$\mathbf{d_s}$= probe size (diameter)

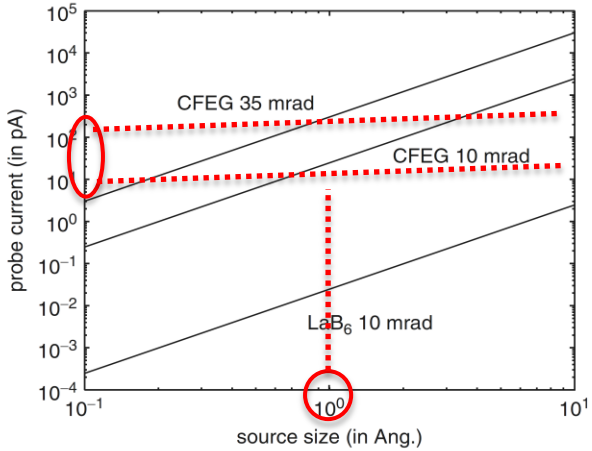
Brightness is conserved in mgentic lenses

Condenser + objective lenses demagnify the image of the source onto the specimen

More source demagnification produces less current

Relation between probe size and probe current

$$I_P = \frac{1}{4}\pi^2\alpha^2\beta d_S^2$$



β= 10^9 amp/(cm²sr)

β= 10^6 amp/(cm²sr)

Each part of the source can emit electrons that can form an image of their own. Each of this image is offset in position and Demgnified by the lenses. →Convolution with an effective source size in the specimen plane

$$g(\mathbf{x}) = f(\mathbf{x}) \otimes h_{\mathrm{ADF}}(\mathbf{x}) \otimes h_{\mathrm{source}}(\mathbf{x})$$

Calculation of Images of Thin specimen

The weak phase object

Primary interaction between electron and specimen → electrostatic potentail and charge of the electron

TEM: incident electrons are a superposition of plane waves

STEM: spherically convergent probe

One plane wave tavelling in z direction

$$\psi(\mathbf{x}) = \exp(2\pi i k_z z) = \exp(2\pi i z/\lambda)$$

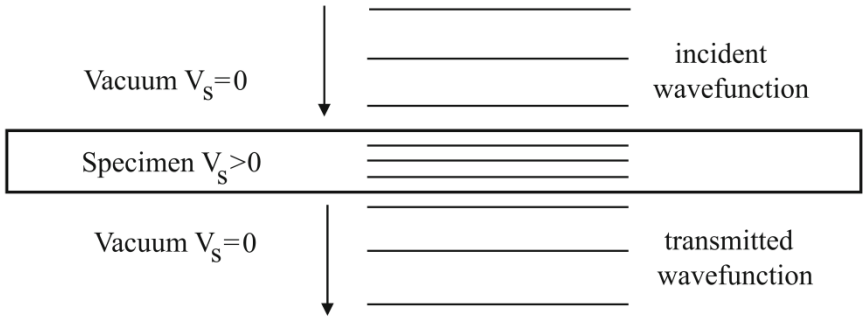
Reciprocal expression for the wave vector in vacuum

$$k_z = \frac{1}{\lambda} = \frac{\sqrt{eV(2m_0c^2 + eV)}}{hc}$$

λ= wavelength of the electron
k_z=1/ λ: propagtion wave vector
h= Planck´s constant
m_0= rest mass of the electron
c= speed of light
eV= kinetic energy of the electron in vacuum
eV_s= kinetic energy of the electron in the specimen

For thin samples electrons pass through the specimen with only a small deviation in their path.

Specimen has a small electrostatic potential. If positive→ electrons are accelerated→ smaller wavelength



$$\frac{1}{\lambda_s} = \frac{[(eV + eV_s)(2m_0c^2 + eV + eV_s)]^{1/2}}{hc}$$
$$= \frac{[eV(2m_0c^2 + eV) + eV_s(2m_0c^2 + 2eV + eV_s)]^{1/2}}{hc}$$
$$= \frac{1}{\lambda}\left[1 + \frac{eV_s(2m_0c^2 + 2eV + eV_s)}{eV(2m_0c^2 + eV)}\right]^{1/2}.$$

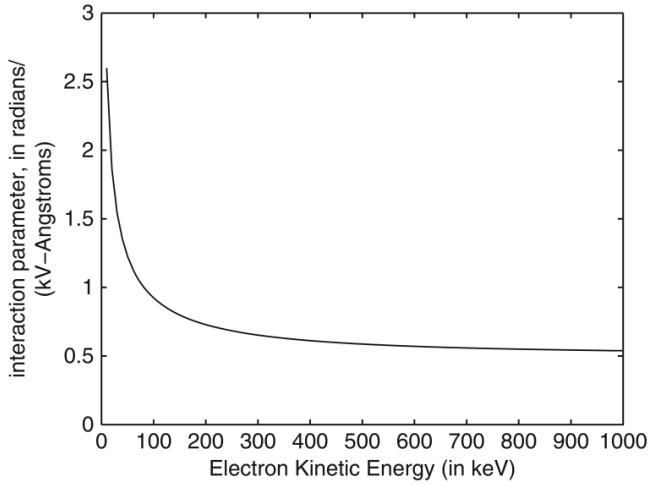
Calculation of Images of Thin specimen

The weak phase object

→ Shift in phase of the electrons → electron wave function in the specimen is:

$$\psi(\mathbf{x}) \sim \exp(2\pi i k_z z)\exp(i\sigma V_s z)$$

$$\sigma = \frac{2\pi}{\lambda V}\left(\frac{m_0c^2 + eV}{2m_0c^2 + eV}\right) = \frac{2\pi m e \lambda}{h^2}$$



σ= interaction parameter
k_z=1/ λ: propagtion wave vector
h= Planck´s constant
m_0= rest mass of the electron ($m=\gamma m_0$)
c= speed of light
eV= kinetic energy of the electron in vacuum
V_s= specimen potential
λ=wavelength
γ=Lorentz factor $\frac{1}{\sqrt{1-\frac{v}{c}}}$
$v_z(x)$= total projected atomic potential

Thin sample: phase shift of the electron wave function is the integral of the potential of the specimen
→ Multiply wave function by transfer function

$$\psi_t(\mathbf{x}) = t(\mathbf{x})\exp(2\pi i k_z z)$$
$$t(\mathbf{x}) = \exp[i\sigma v_z(\mathbf{x})]$$

$$v_z(\mathbf{x}) = v_z(x,y) = \int V_s(x,y,z)\mathrm{d}z$$

→ Weak phase object approximation

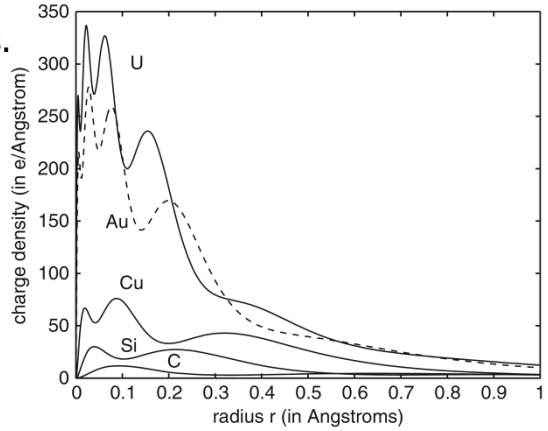
Calculation of Images of Thin specimen

Single atom properties

Radial Electron Charge Distribution

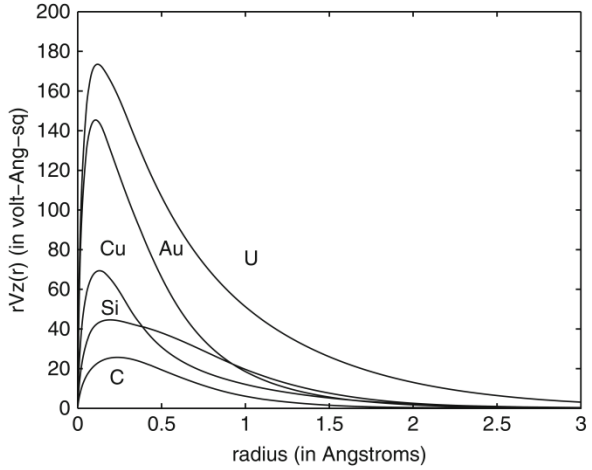
The peaks correspond to the atomic orbitals.

Electron cloud shields the atomic nucleus

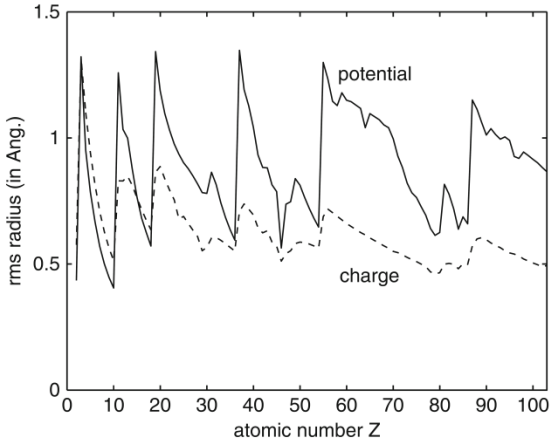


Atomic sizes

Projected Potential multiplied by the radius r to illustrate the Relative contribution to an image



The rms radius of isolated single atoms as determined from the (3D) potential charge and the (2D) projected atomic potential



Calculation of Images of Thin specimen

Single atom properties

Potential

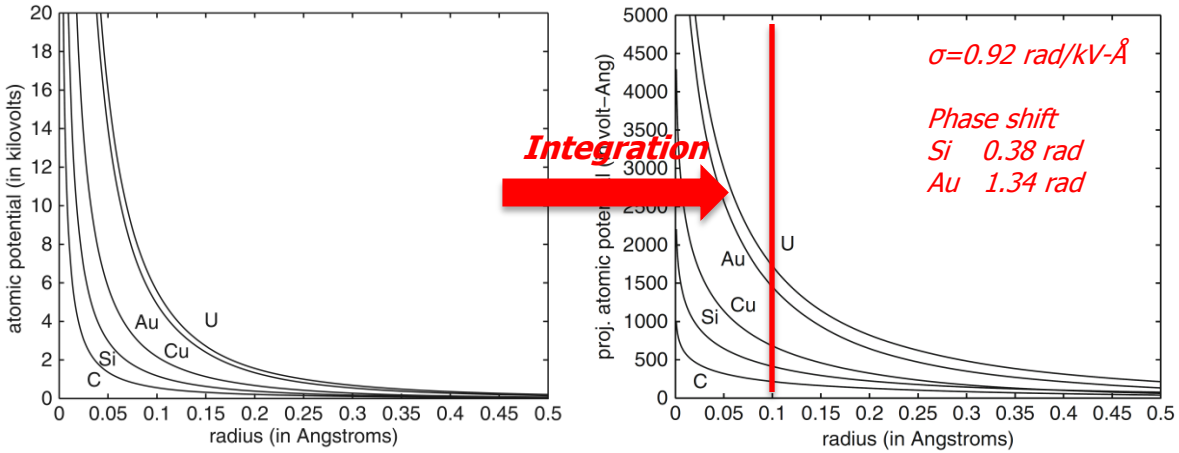
Electrons in the microscope interact directly with the atomic potential

Charge distribution and potential are related vie Poisson´s equation from electromagnetic theory

The charge distribution only includes the electron charge distribution.

The large point charge on the atomic nucleus has the strongest interaction with the imaging electrons.

Addition of nucleus to electron charge distribution + transforming into an atomic potential → much more peaked at the nucleus



→ *Si is reasonable weak*
Au not

$$\psi_t(\mathbf{x}) \sim t(\mathbf{x}) \sim \exp[\mathrm{i}\sigma_e v_z(\mathbf{x})] \sim 1 + \mathrm{i}\sigma_e v_z(\mathbf{x}) + \cdots$$

All atoms have a near singularity at a radius close to 0; so no atom is truly a WPO in a strict sense.

Calculation of Images of Thin specimen

The scattering factor

Electron scattering: outgoing plane wave + outgoing spherical wave (spherical symmetry of the atoms) with amplitude ($f_e(q)$)

$$\psi(\mathbf{x}) = \exp(2\pi i k_z z) \quad \text{incident}$$
$$= \exp(2\pi i k_z z) + f_e(q)\frac{\exp(2\pi i \mathbf{q}\cdot\mathbf{r})}{r} \quad \text{scattered}$$

q= 3D wave vector (difference between incident and scattered wave)

Born approximation:

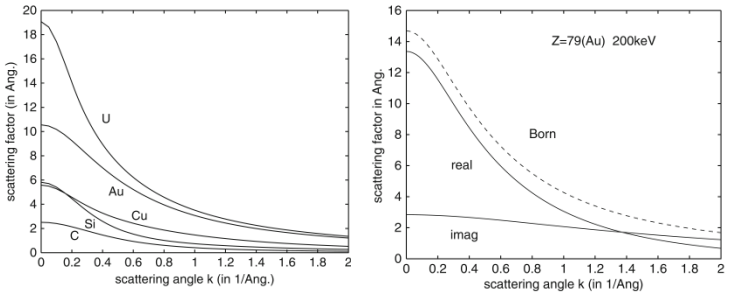
$$f_e(q) = \frac{1}{\pi e a_0 q}\int_0^\infty V_a(r)\sin(2\pi q r) r\,dr.$$

a_0= Bohr radius (0.5292Å)
$V_a(r)$= 3D atomic potential of the atom
e= magnitude of the charge of the electron

Amplitude of a single electron scattered by single atom

Inadequate for directly calculating electron scattering in the EM, but usful for calculating the specimen potential

$f_e(q)$ should be complex; elastic scattering: should be destroyed or created



Moliere approximation:

$$f_e(q) = \frac{2\pi i}{\lambda}\int_0^\infty J_0(2\pi q r)\left\{1 - \exp\left[i\sigma\int V(x,y,z)dz\right]\right\} r\,dr$$

J_0= Bessel function of 0. order
σ= interaction parameter
λ= wavelength

Calculation of Images of Thin specimen

The specimen potential

Electrons interact with the specimen as a whole.

Simulation requires the knowledge of the position of all atoms

Linear superposition approximation of the potentials of each atom in the specimen

$$v_z(\mathbf{x}) = \sum_{j=1}^{N} v_{zj}(\mathbf{x} - \mathbf{x}_j)$$

$\mathbf{x_j} = (\mathbf{x_j}, \mathbf{y_j})$: position of atom j
$\mathbf{v_{zj}(x)}$: projected atomic potential of the atom

Exact for seperated atoms

Solids: atoms are bound together and outer electrons rearrange slightly

Slight change in **$\mathbf{v_{zj}}$**

In ADF-STEM: high angle scattering occures at atomic nucleus which by bonding

No influence on the linear superposition approximation.

From the specimen potential and the scattering factor the **structure factor** can be calculated:

$$F(\mathbf{q}) = \sum_j f_{ej}(\mathbf{q}) \exp(2\pi i \mathbf{q} \cdot \mathbf{x}_j)$$

q= 3D wave vector (difference between incident and scattered wave)

Calculation of Images of Thin specimen

BF phase contrast image calculation

Remember: BF-TEM and BF-STEM are connected via the reciprocity theorem.

Incident electron wave function is a single plane wave of unit intensity

Interaction wit hspecimen → phase shift which is position dependent → specimen transfer function

$$\psi_t(\mathbf{x}) = t(\mathbf{x}) \exp(2\pi \mathrm{i} k_z z) \sim t(\mathbf{x})$$

$$t(\mathbf{x}) = \exp\left[\mathrm{i}\sigma v_z(\mathbf{x})\right]$$

$v_z(x)$= total projected atomic potential
σ= interaction parameter
k_z= wave vector in z direction

Transmitted wave function imaged by the objective lens

$$\Psi_t(k) = \mathrm{FT}[\psi_t(\mathbf{x})]$$
$$\Psi_i(k) = \Psi_t(\mathbf{k}) H_0(\mathbf{k})$$

$$H_0(\mathbf{k}) = \exp[-\mathrm{i}\chi(\mathbf{k})] A(\mathbf{k})$$
$$\chi(k) = \pi\lambda k^2 (0.5 C_s \lambda^2 k^2 - \Delta f)$$
$$A(\mathbf{k}) = 1; \quad \lambda k = \alpha < \alpha_{\max}$$
$$= 0; \quad \text{otherwise}$$

$\Psi i(k)$= image wave function in the back focal plane
$H_0(k)$= transfer function of the objective lens
$\chi(k)$= abberation function
$A(k)$= aperture function
Δf= defocus
C_s= spherical aberration
α_{max}= maximum semiangle of the objective aperture

Actual recorded image is the magnitude squared of the image wave function after inverse FT back to real space

$$\psi_i(\mathbf{x}) = \mathrm{FT}^{-1}[\Psi_i(\mathbf{k})]$$
$$g(\mathbf{x}) = |\psi_i(\mathbf{x})|^2 = |\psi_t(\mathbf{x}) \otimes h_0(\mathbf{x})|^2$$

$h_0(x)$= complex point spread function of the objective lens

Calculation of Images of Thin specimen

Steps in the calculation of CTEM images

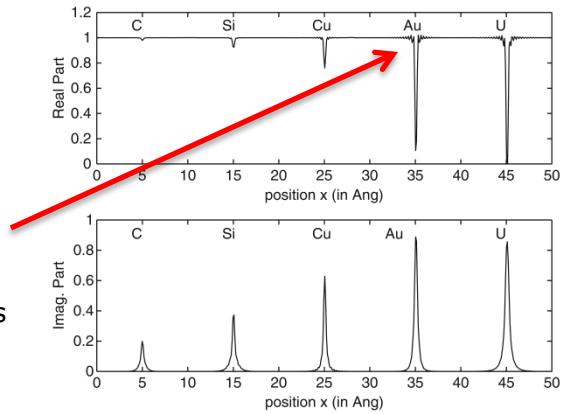
Step 1	Calculate the projected atomic potential $v_z(\mathbf{x})$ from (5.19) or (5.21).
Step 2	Calculate the transmission function $t(\mathbf{x}) = \exp[i\sigma v_z(\mathbf{x})]$ (5.25) and symmetrically bandwidth limit it. The incident wave function is a plane wave so the transmitted wave function is equal to the transmission function.
Step 3	Fourier transform the transmission function $T(\mathbf{k}) = \mathrm{FT}[t(\mathbf{x})]$.
Step 4	Multiply the Fourier transform of the transmission function by the transfer function of the objective lens, $H_0(k)$ (5.27) to get the image wave function in the back focal plane $\Psi_i(\mathbf{k}) = H_0(k)T(\mathbf{k})$.
Step 5	Inverse Fourier transform the image wave function $\psi_t(\mathbf{k}) = \mathrm{FT}^{-1}[\Psi_i(\mathbf{k})]$.
Step 6	Calculate the square modulus of the image wave function (in real space) to get the final image intensity $g(\mathbf{x}) = \lvert\psi_t(\mathbf{x}) \otimes h_o(\mathbf{x})\rvert^2$.

Calculation of Images of Thin specimen

Single Atoms Images

Specimen transmission function:

Slight ringing near the atoms:
Finite bandwith
+
Slight asymmetry:
Some atome positions are not exctly integer
With pixel size



Atom´s distance: 10 Å
Image size: 50 Å
512 x 512 pixels
Atomic potential where calculated
The Moliere apporximation

Real part depends stronger on the atomic number Z than the imaginary part.

Remember: potential has a singularity for r=0 (center of the atom)

Value at the center of the atom: average over one pixel

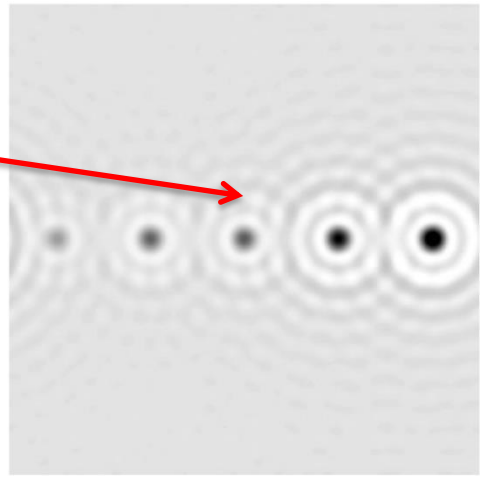
→ Smaller pixel size leads to values closer to the singular value at the center

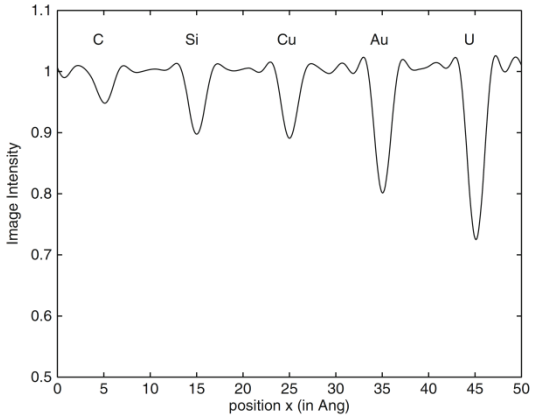
Image intensity:

Image intensity between the atoms should be one (vacuum)

Rings are part of the Airy disk due to sharp cut off in reciprocal space due to the objective aperture

Rings on the right wrap around to interfere with the atom on the left (wrap-around effect)





Line scan through the center

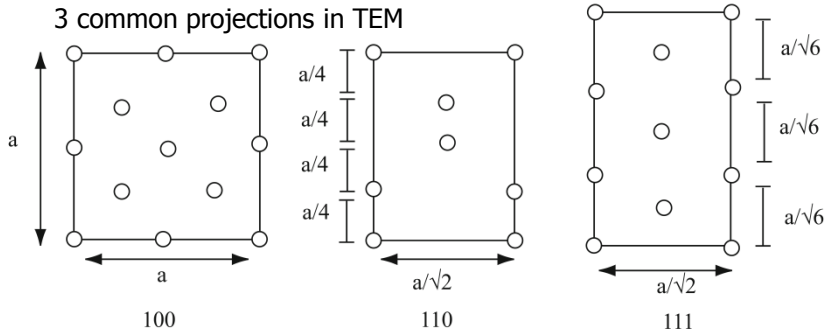
T. Lunkenbein, FHI

Calculation of Images of Thin specimen

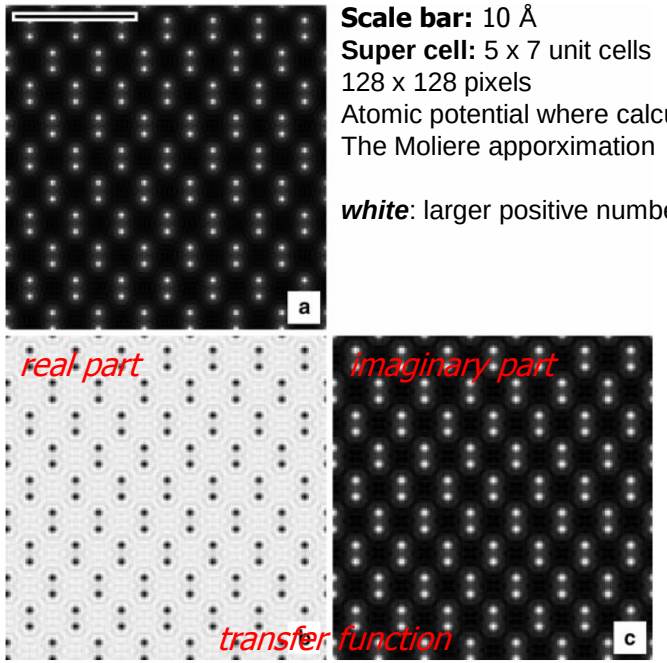
Thin specimen images

Example: Si

low atomic number →WPO
Simple fcc structure



Projected atomic potential of a 4 atoms thick (110) Si



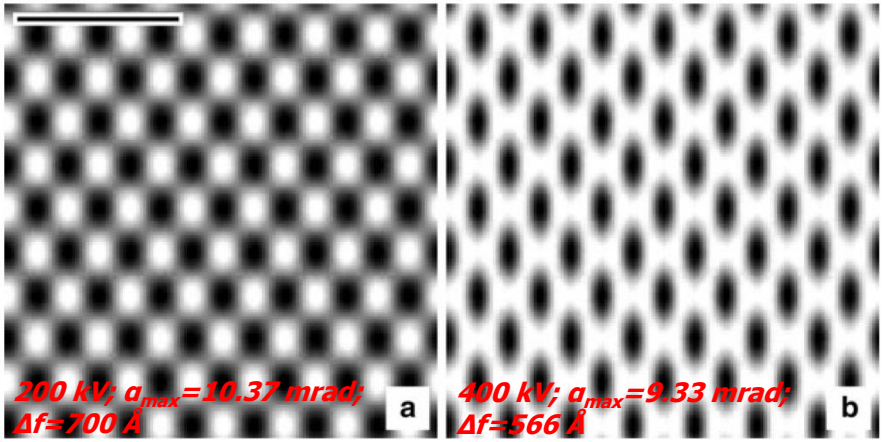
Scale bar: 10 Å
Super cell: 5 x 7 unit cells
128 x 128 pixels
Atomic potential where calculated
The Moliere apporximation

white: larger positive number

Calculation of Images of Thin specimen

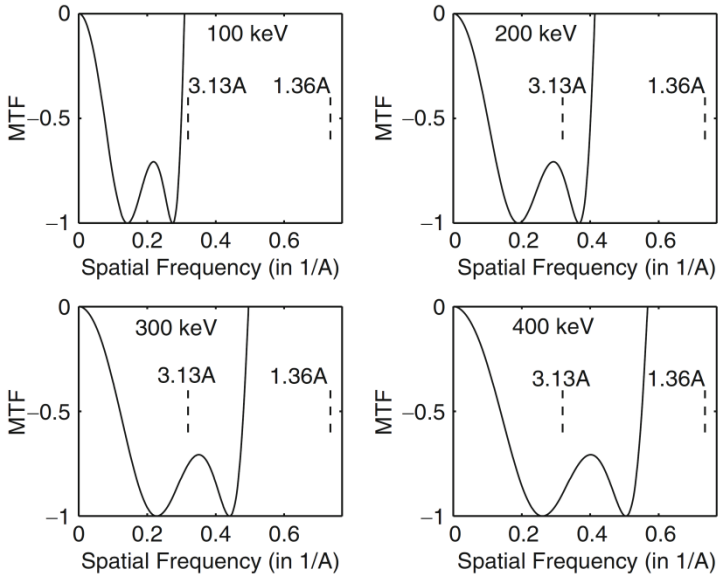
Thin specimen images

Coherent BF images of (110) Si in the WPO approximation



Scale bar: 10 Å
Super cell: 5 x 7 unit cells
128 x 128 pixels
Scherzer conditions
white: larger positive number; atoms should appear black

Transfer function for a coherent BF image of (110) Si in the WPO approximation



T. Lunkenbein, FHI

Calculation of Images of Thin specimen

ADF STEM images of thin specimen

Objective lens is before the specimen (see reciprocity theorem)

Transmitted electrons get scattered at high angles to form the ADF signal

Wave function of the focused probe incident upon the specimen at position xp is the integral of the aberration wave function over the objective aperture:

$$\psi_p(\mathbf{x},\mathbf{x}_p) = A_p \int_0^{k_{\max}} \exp[-\mathrm{i}\chi(\mathbf{k}) - 2\pi\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}_p)]\mathrm{d}^2\mathbf{k},$$

$\lambda k_{max}=\alpha$: maximum angle in the objective aperture
A_p: normalization constant

Specimen transfer function:

$$\begin{aligned}\psi_t(\mathbf{x},\mathbf{x}_p) &= \psi_p(\mathbf{x},\mathbf{x}_p)t(\mathbf{x}) \\ &= \psi_p(\mathbf{x},\mathbf{x}_p)\exp[i\sigma v_z(\mathbf{x})]\end{aligned}$$

σ= interaction parameter
$v_z(x)$= total projected atomic potential

Transmitted wave function is diffracted into the far field and hits the detector

$$\Psi_t(\mathbf{k}) = \mathrm{FT}[\psi_t(\mathbf{x})].$$

The detector integrates the square modulus of the wave function in the diffraction plane to form the ADF-STEM at this point in the image

$$g(\mathbf{x}_p) = \int D(\mathbf{k})|\Psi_t(\mathbf{k},\mathbf{x}_p)|^2\mathrm{d}^2\mathbf{k},$$

D(k)= detector function

$$\begin{aligned}D(\mathbf{k}) &= 1 \quad \text{on the detector} \\ &= 0 \quad \text{otherwise.}\end{aligned}$$

Probe scans across the specimen → process is repeated for each new position

Detector: large annulus covering only high angle scattering

Calculation of Images of Thin specimen

Steps in the calculation of ADF-STEM images

Step 1	Calculate the projected atomic potential $v_z(\mathbf{x})$ from (5.19) or (5.21).
Step 2	Calculate the transmission function $t(\mathbf{x}) = \exp[\mathrm{i}\sigma v_z(\mathbf{x})]$ (5.25) and symmetrically bandwidth limit it.
Step 3	Calculate the probe wave function $\psi_p(\mathbf{x}, \mathbf{x}_p)$ at position $\mathbf{x}_p$ (5.45,5.47)
Step 4	Multiply the probe wave function by the specimen transmission function $t(\mathbf{x}) = \exp[\mathrm{i}\sigma v_z(\mathbf{x})]$ to get the transmitted wave function $\psi_t(\mathbf{x})$.
Step 5	Fourier transform the transmitted wave function to get the wave function in the far field (diffraction plane).
Step 6	Integrate the intensity (square modulus) of the wave function in the diffraction plane including only those portions that fall on the annular detector (5.50). This is the signal for one point or pixel in the image.
Step 7	Repeat step 3 through step 6 for each position of the incident probe $\mathbf{x}_p$.

Calculation of Images of Thin specimen

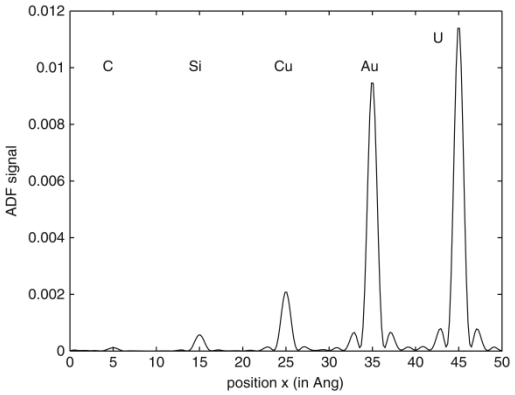
ADF STEM: Single atom images

Specimen transfer function the same than in BF-TEM

ADF is relative to the incident beam current
BF relative to the incident beam current density (incident beam has uniform intensity at all positions)

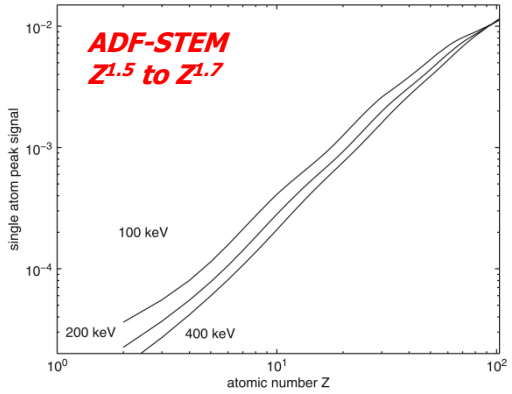
ADF signal much weaker than the BF singal

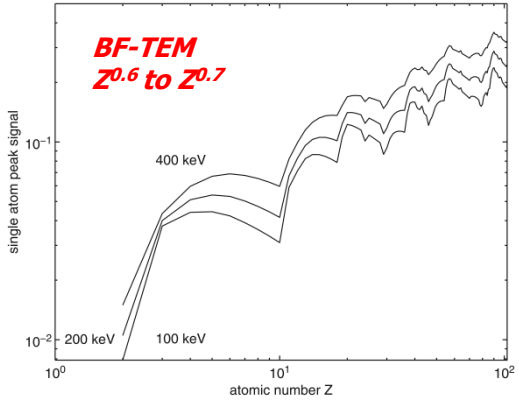
Line scan through the center



ADF image shows higher contrast between light and heavy atoms

Peak single atom signal ADF-STEM vs. BF-TEM

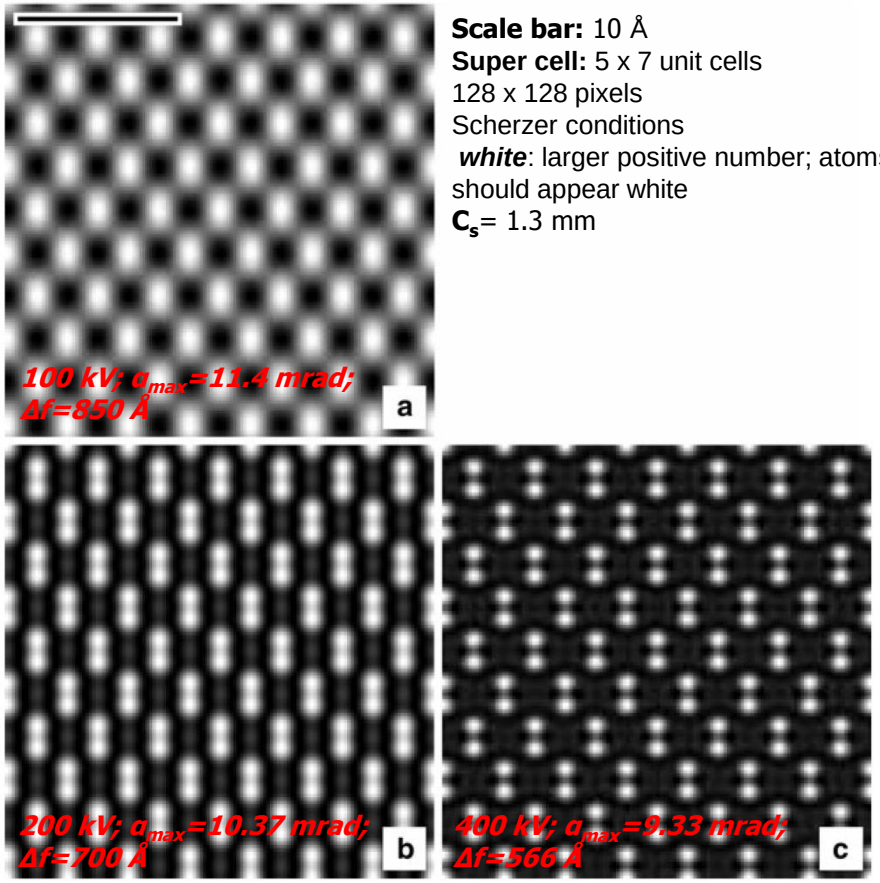




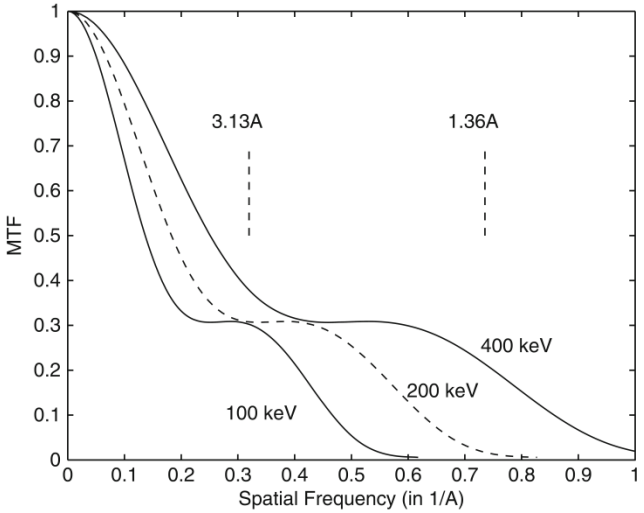
Calculation of Images of Thin specimen

ADF STEM: Thin specimen images

Simulated ADF-STEM images of (110) Si (4 atoms thick) in the WPO approximation



Scale bar: 10 Å
Super cell: 5 x 7 unit cells
128 x 128 pixels
Scherzer conditions
white: larger positive number; atoms should appear white
$\mathbf{C_s}$= 1.3 mm

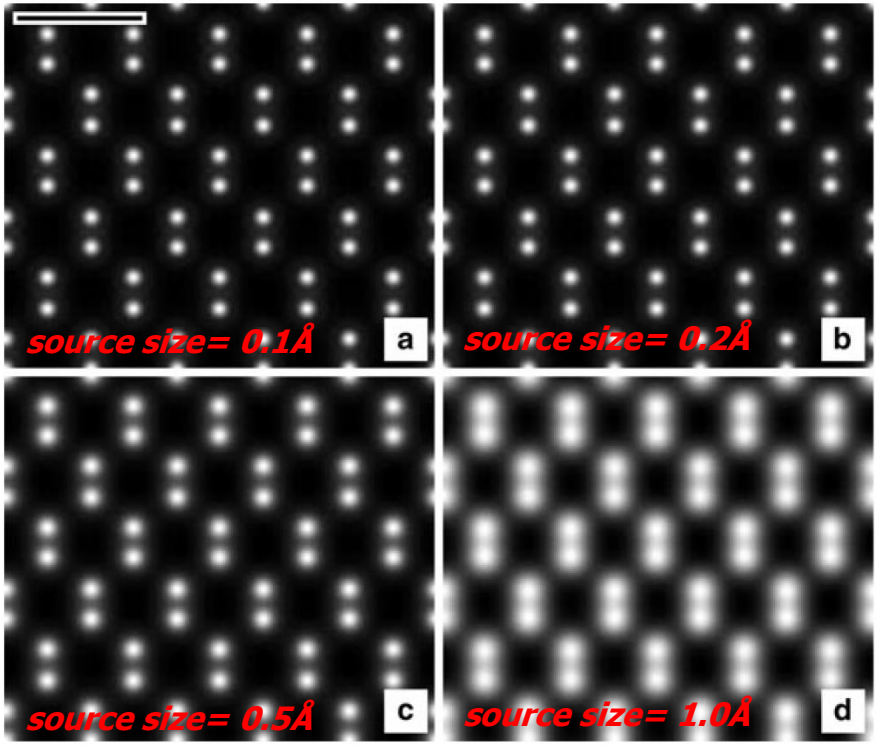


Transfer function for an inchorrent ADF-STEM image under Scherzer conditions

Calculation of Images of Thin specimen

ADF STEM: Thin specimen images

Simulated ADF-STEM images of (110) Si (4 atoms thick) in the WPO approximation at 100keV



Scale bar: 5 Å
Super cell: 5 x 7 unit cells
white: larger positive number; atoms should appear white
$\mathbf{C_s}$= 0 mm
$\mathbf{\alpha_{max}}$=35 mrad
Δf=0 Å

Calculation of Images of Thick Specimens

ADF STEM: Thin specimen images

Tick samples: multiple + geometric extention along the optical axis

→ Electron interacts strongly with the sample and can scatter more than once → dynamic scattering

Instrumental aspects: electron microscope + the passage of the elctrons through the microscope are the same

Only difference: specimen

Shortest part, but the most difficult part to calculate, because of the strong interaction of the elctrons with the specimen

2 Theories:

Bloch wave

Wave function of a particle in periodically repeating potential

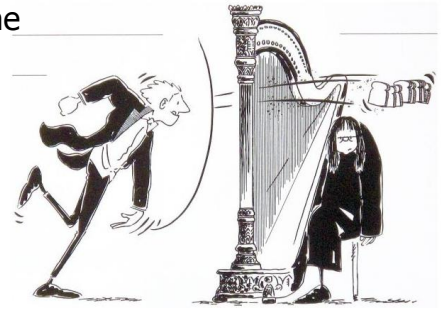
1928: Bethe solved 3D eigenvalues of the electron wave funvtion in a crystalline specimen
Using appropiate boundary conditions on the entrance and exit face of the crystal

Mulitslice Method

Specimen divided into thin 2D slices along z

Electron beam gets transmitted through a slice and propagates to the next slice

Each slice is thin enough to be a simple phase object and the propagation between slices is determined by Frsenel diffraction



Simulation Programs lead to wide spread use of simulation in HR image interpreatation

Calculation of Images of Thick Specimens

Bloch waves:

Electron wave function can be expressed by a linear combination of any complete basis set

Using a basis set that also satisfies the Schrödinger equation in the specimen (periodic crystal) are called Bloch waves)

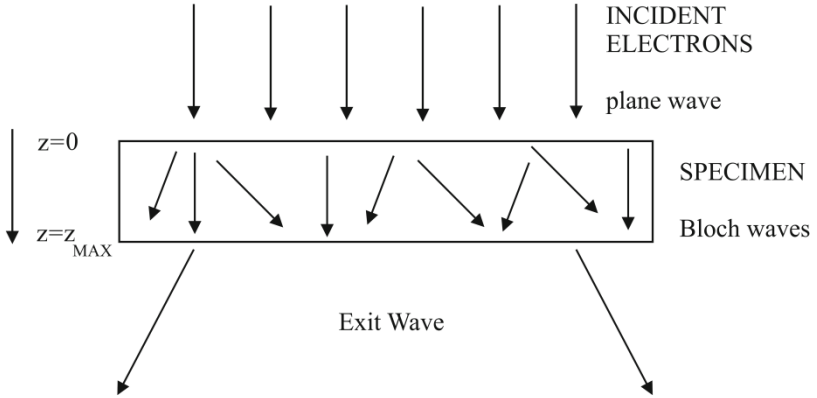
$$\psi(x,y,z) = \psi(\mathbf{r}) = \sum_j \alpha_j b_j(\mathbf{k}_j, \mathbf{r})$$

$b(\mathbf{k}_j, \mathbf{r})$ Expansion of the electron wave Function to Bolch waves

kj: scattering vector on the Ewald sphere

With these Bloch waves any set of coefficients αj are allowed inside the crystal, BUT only one set will also match the incident wave function

Specimen: converter or filter that converts the incident electrons into a superposition of Bloch waves inside the specimen



Characteristics of this Bloch waves determine how the electrons travel through the sample.

Calculation of Images of Thick Specimens

Steps in the Bloch wave eigenvalue calculation:

Each Bloch wave must satisfy the Schrödinger equation and is forced to have the periodicity of the specimen:

$$b_j(\mathbf{k}_j,\mathbf{r}) = \exp[2\pi i\mathbf{k}_j\cdot\mathbf{r}]\sum_{\mathbf{G}} C_{\mathbf{G}j}\exp[2\pi i\mathbf{G}\cdot\mathbf{r}]$$
$$= \sum_{\mathbf{G}} C_{\mathbf{G}j}\exp[2\pi i(\mathbf{k}_j+\mathbf{G})\cdot\mathbf{r}].$$

(1) Calculate the Fourier coefficient (V_G) of the atomic potential V(r)

h= Planck´s constant
m_0= relativistic mass of the elctron
e= magnitude of the charge of the electron
a_0= Bohr´s atomic radius
F_{ej}= electron scattering factor in the first Born approximation
Ω= unit cell volume
j= all atoms in the unit cell
G=(G_x,G_y,G_z)= (h/a, k/b, l/c): reciprocal lattice Vectors
C_{Gj}= set of coefficient for each Bloch wave j

$$V(x,y,z) = V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}}\exp[2\pi i\mathbf{G}\cdot\mathbf{r}]$$

3D- Fourier series

$$V_{\mathbf{G}} = \frac{h^2}{2\pi m_0 e}\frac{1}{\Omega}\sum_j f_{ej}(|\mathbf{G}|)\exp(-2\pi i\mathbf{G}\cdot\mathbf{r}_j)$$
$$= \frac{2\pi e a_0}{\Omega}\sum_j f_{ej}(|\mathbf{G}|)\exp(-2\pi i\mathbf{G}\cdot\mathbf{r}_j)$$
$$= \frac{47.86}{\Omega}\sum_j f_{ej}(|\mathbf{G}|)\exp(-2\pi i\mathbf{G}\cdot\mathbf{r}_j),$$

When the crystal has a symmetry center → for every atom at position r there is an identical atom at position –r and The terms appear as pairs of complex conjugates making VG real, if not it is complex.

Calculate all VG up to some maximum magnitude of G (scan through integers (h,k,l) and keep all with $|V_G| > \varepsilon|V_{G=0}|$; $\varepsilon \sim 10^{-5}$

Calculation of Images of Thick Specimens

Bloch waves:

(2) Solve for the eigenvalues (proportional to γ_j) and eigenvectors C_G:

$$2k_0 s_{\mathbf{G}} C_{\mathbf{G}j} + \sum_{\mathbf{H}\neq\mathbf{G}} U_{\mathbf{G}-\mathbf{H}} C_{\mathbf{H}j} = 2\gamma_j k_{0,z} C_{\mathbf{G}j}$$

$\mathbf{s_G}$= excitation error
$\boldsymbol{\gamma_j}$ = small term along the beam direction
C= matrix
j= all atoms in the unit cell
G=(G_x,G_y,G_z)= (h/a, k/b, l/c): reciprocal lattice Vectors
C_{Gj}= set of coefficient for each Bloch wave j
α_j=weighting coefficient

(3) Find the weighting coefficients α_j to match the incident wave function at z=0

$$\mathrm{C}^{-1}\psi(z=0) = \mathrm{C}^{-1}\mathrm{C}\alpha = \alpha$$
$$\alpha = \mathrm{C}^{-1}\psi(z=0) = \mathrm{C}^{\dagger}\psi(z=0)$$

$$\begin{bmatrix} \psi_0(z) \\ \psi_D(z) \\ \psi_E(z) \\ \psi_F(z) \end{bmatrix} = \begin{bmatrix} C_{00} & C_{01} & C_{02} & C_{03} \\ C_{D0} & C_{D1} & C_{D2} & C_{D3} \\ C_{E0} & C_{E1} & C_{E2} & C_{E3} \\ C_{F0} & C_{F1} & C_{F2} & C_{F3} \end{bmatrix} \times \begin{bmatrix} e^{2\pi i\gamma_0 z} & 0 & 0 & 0 \\ 0 & e^{2\pi i\gamma_1 z} & 0 & 0 \\ 0 & 0 & e^{2\pi i\gamma_2 z} & 0 \\ 0 & 0 & 0 & e^{2\pi i\gamma_3 z} \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix}$$

(4) Calculate the electron wave function at the exit surface of the specimen

column vector $\quad \psi(z) = \mathrm{C}[\exp(2\pi i\gamma_j z)]\alpha$

$$\psi(x,y,z) = \mathrm{FT}_{xy}^{-1}\left[\sum_{\mathbf{G}} \psi_{\mathbf{G}} \exp(2\pi i G_z z)\right]$$

$$\frac{\partial\phi_{\mathbf{G}}(z)}{\partial z} = -\pi i(2G_z + \lambda G_x^2 + \lambda G_y^2)\phi_{\mathbf{G}}(z) + i\sigma\sum_{\mathbf{G}'} V_{\mathbf{G}-\mathbf{G}'}\phi_{\mathbf{G}'}(z)$$
$$= 2\pi i s_{\mathbf{G}}\phi_{\mathbf{G}}(z) + i\sigma\sum_{\mathbf{G}'} V_{\mathbf{G}-\mathbf{G}'}\phi_{\mathbf{G}'}(z).$$

Calculation of Images of Thick Specimens

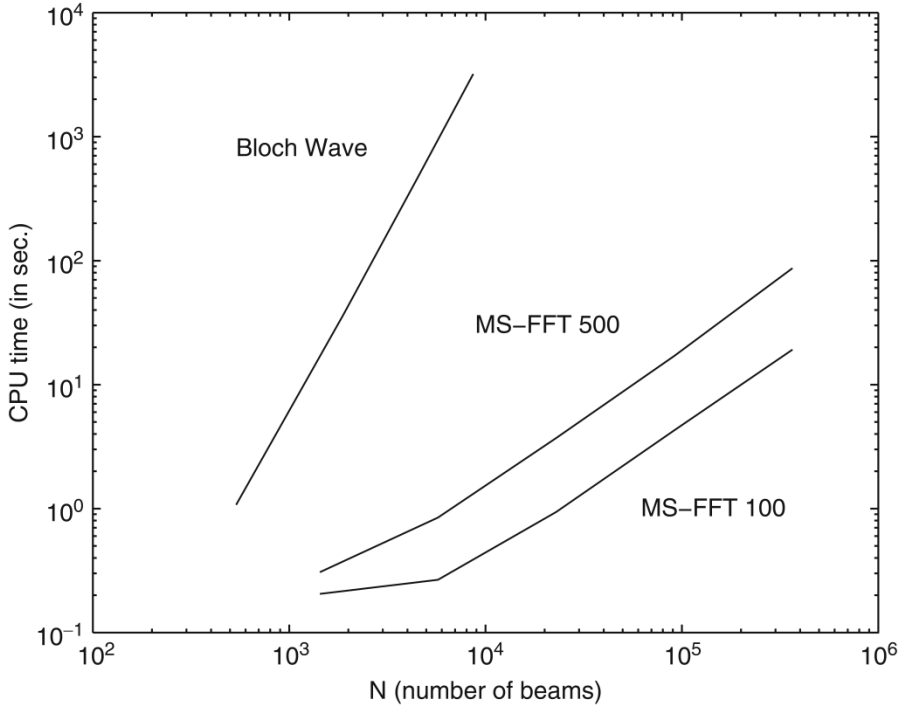
Bloch waves:

Limitations:

The computer time requiered for a matrix multiplication scales as N^2 for the direct solution of a matrix

Large number of beams (>20) a direct matrix (Bloch wave) solution becomes very inefficient

Only 2 or 3 Bloch waves (beams) should be involved → specimen is a perfect crystal with a small unit cell



Calculation of Images of Thick Specimens

Multislice Solution

Let´s start simple:

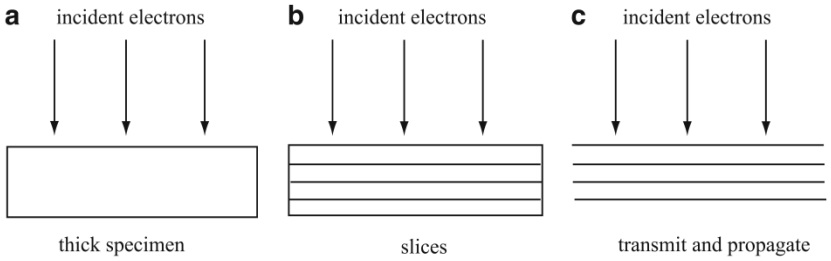
$$\psi_{n+1}(x,y) = t_n(x,y)\,[p_n(x,y,\Delta z_n) \otimes \psi_n(x,y)] + \mathcal{O}(\Delta z^2)$$

wave function at the top of each slice

transmission function

propagation function

incident plane wave



At each slice the electron wave function experiences a phase shift due the projected atomic potential of all atoms And then propagates.

Each slice is idependent of all other slices (slice thickness and transmission function may vary.

Calculation of Images of Thick Specimens

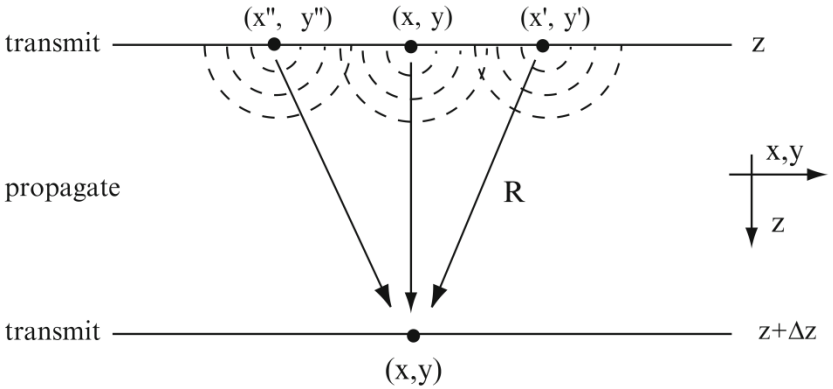
Multislice Solution – Physical optics viewpoint

The propagator function can be associated with the Fresenel (near zone) diffraction over a distance Δz

Huygens´principle states that every point of a wave front gives rise to an outgoing spherical wave.

These outgoing spherical waves propagate to the next position of the wavefront and interfere with one another.

The wave function in an x, y plane at z+ Δz is the interference of all of these spherically outgoing waves that originated in an x,y plane at z.



This propagation of the wave front can be calculated by the Fresnel Kirchhoff diffraction integral

$$\psi(x,y,z+\Delta z) = \frac{1}{2i\lambda}\int \psi(x',y',z)\frac{\exp(2\pi iR/\lambda)}{R}(1+\cos\theta)\mathrm{d}x'\mathrm{d}y', \qquad R=\sqrt{(x-x')^2+(y-y')^2+\Delta z^2}$$

$$p(x,y,\Delta z) = \frac{1}{\mathrm{i}\lambda\Delta z}\exp\left[\frac{i\pi}{\lambda\Delta z}(x^2+y^2)\right]$$

The mulitslice propagator function can be interpreted simply as the Fresnel diffraction over a distance $\Delta z = \Delta f$.

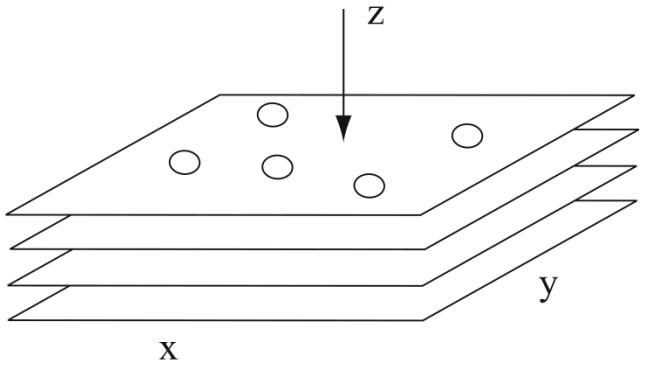
Calculation of Images of Thick Specimens

Slicing the specimen

Slicing the specimen in a form that it can be used in the multislice program (rectangular)→ most difficult part

The specimen must be described as a sequence of layers and spacings in the program.

Each slice must be thin enough to be a weak phase object and perpendicular to the obtical axis



All of the atoms within z to z+ Δz are compressed into flat planeor slize at z.

Slice must be aligned with natural periodicity + the edges of the slice (in x,y plane) must have periodic boundary conditions (in x and y) → Wrap around effect

Many crystalline specimen have identical atomic layers (e.g. (111) Si: stacking sequence of abcabc....)

Calculation of Images of Thick Specimens

Slicing the specimen

Aligning the natural atomic layers of the specimen with the slices can have beneficial side effects.

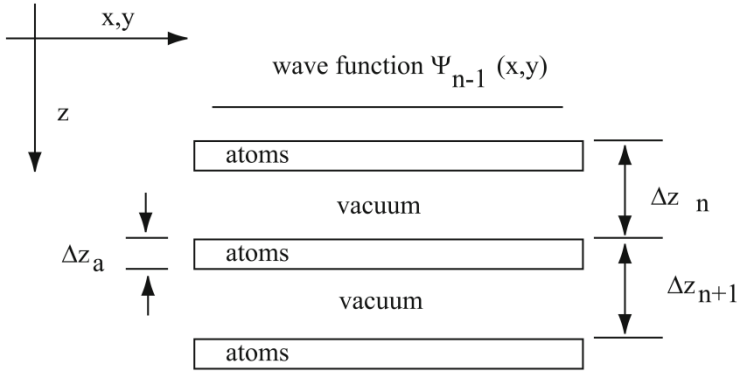
The atomic potential peaks at the nucleus (singularity) and falls off quickly (1/r dependence)

→The effective range of the potential in the atoms can be smaller than the distance in the layer

The potential is identically 0 in between the layers (vacuum). The transmission in vacuum is nearly exact → the error occurs only over the thickness of the layer:

$$p(x,y,\Delta z) = p(x,y,\Delta z - \Delta z_a) \otimes p(x,y,\Delta z_a)$$

Multislice equation: transmission + propagator over Δz_a followd by a propagation over a distance $\Delta z - \Delta z_a$.
The effective error is of order Δz_a → significantly smaller than total slice thickness Δz.



Calculation of Images of Thick Specimens

Table 6.2 Some image simulation software packages appearing in the literature or on-line

Program	Author	Year	Type	Comments
SHRLI	O'Keefe and Buseck [269]	1978,9	M	
TEMPAS	Kilaas [194]	1987	M	
EMS	Stadelmann [335]	1987	B	
NCEMSS	O'Keefe and Kilaas [271]	1988	M	
MacTEMPAS	Kilaas [195]	?	M	on-line
TEMSIM	Kirkland [205]	1998	M	CD, on-line
?	Ishizuka [178]	2001	B, M	online
?	deGraf [129]	2003	B	online
JEMS	Stadelmann [336]	2004	B, M	online
WebEMAPS	Zuo [334, 393]	2005	B	online
EDM	Marks et al [235]	2006	B,M	online
SimulaTEM	Gómez-Rodríguez et al. [123]	2010	M	online

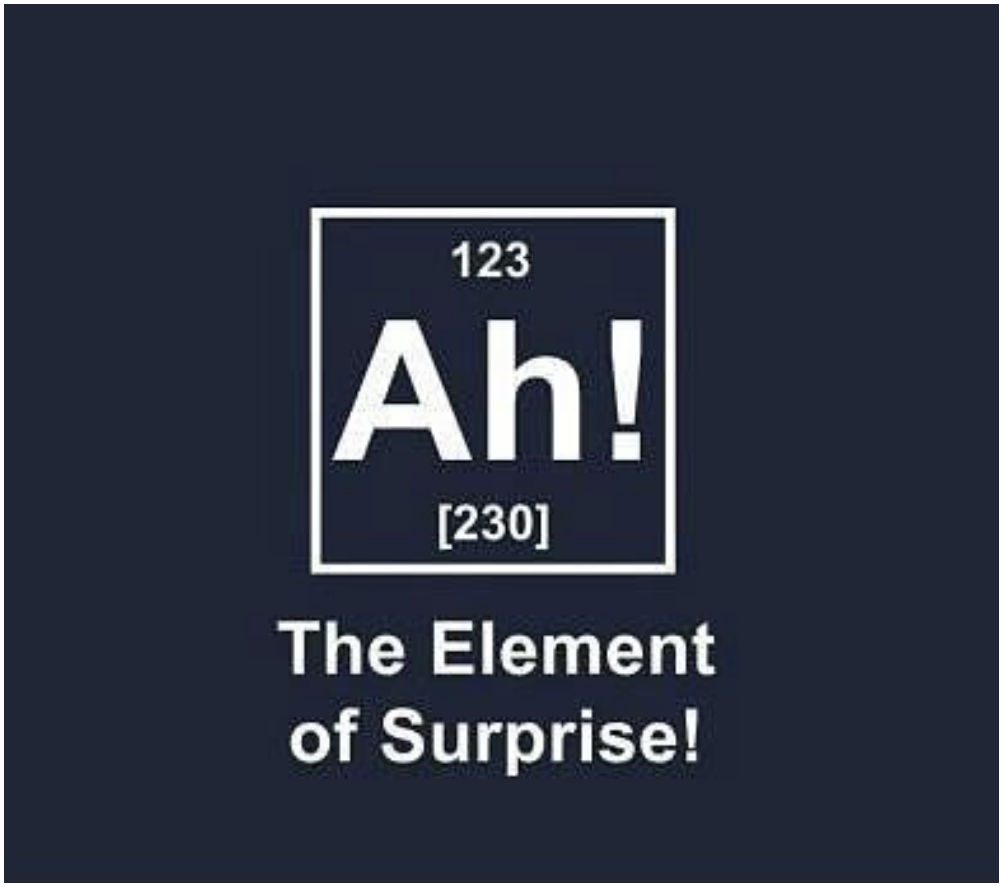
Type M is multislice and type B is Bloch-Wave. Some of the listed programs may be commercial. Many other private programs likely exist

Table 6.3 Steps in the simulation of CTEM images of thick specimens

Step 1	Divide the specimen into thin slices.
Step 2	Calculate the projected atomic potential $v_{zn}(\mathbf{x})$ [(5.19) or (5.21)] for each slice and symmetrically bandwidth limit them.
Step 3	Calculate the transmission function $t_n(\mathbf{x}) = \exp[i\sigma v_{zn}(\mathbf{x})]$ (5.25) for each slice and symmetrically bandwidth limit each to 2/3 of it maximum to prevent aliasing.
Step 4	Initialize the incident wave function $\psi_0(x,y) = 1$.
Step 5	Recursively transmit and propagate the wave function through each slice $\psi_{n+1}(x,y) = p_n(x,y,\Delta z_n) \otimes [t_n(x,y)\psi_n(x,y)]$ using FFT's as in (6.92). Repeat until the wave function is all the way through the specimen
Step 6	Fourier transform the wave function at the exit surface of the specimen $\Psi_n(k_x,k_y) = \mathrm{FT}[\psi_n(x,y)]$.
Step 7	Multiply the transmitted wave function $\Psi_n(k_x,k_y)$ by the transfer function of the objective lens, $H_0(k)$ (5.27) to get the image wave function in the back focal plane $\Psi_i(\mathbf{k}) = H_0(k)\Psi_n(\mathbf{k})$.
Step 8	Inverse Fourier transform the image wave function $\psi_i(\mathbf{x}) = \mathrm{FT}^{-1}[\Psi_i(\mathbf{k})]$.
Step 9	Calculate the square modulus of the image wave function (in real space) to get the final image intensity $g(\mathbf{x}) = \lvert\psi_i(\mathbf{x})\rvert^2 = \lvert\psi_n(\mathbf{x}) \otimes h_o(\mathbf{x})\rvert^2$.

Table 6.4 Steps in the simulation of STEM images of thick specimens

Step 1	Divide the specimen into thin slices.
Step 2	Calculate the projected atomic potential $v_{zn}(\mathbf{x})$ [(5.19) or (5.21)] for each slice and symmetrically bandwidth limit them.
Step 3	Calculate the transmission function $t_n(\mathbf{x}) = \exp[i\sigma v_{zn}(\mathbf{x})]$ (5.25) for each slice and symmetrically bandwidth limit each to 2/3 of it maximum to prevent aliasing.
Step 4	Calculate the probe wave function $\psi_p(\mathbf{x},\mathbf{x}_p)$ at position $\mathbf{x}_p$ (5.45,5.47)
Step 5	Recursively transmit and propagate the probe wave function through each slice $\psi_{n+1}(x,y) = p_n(x,y,\Delta z_n) \otimes [t_n(x,y)\psi_n(x,y)]$ using FFT's as in (6.92). Repeat until the wave function is all the way through the specimen
Step 6	Fourier transform the transmitted wave function to get the wave function in the far field (diffraction plane).
Step 7	Integrate the intensity (square modulus) of the wave function in the diffraction plane including only those portions that fall on the detector (5.50). This is the signal for one point or pixel in the image.
Step 8	Repeat step 4 through step 7 for each position of the incident probe $\mathbf{x}_p$.


123
Ah!
[230]
The Element
of Surprise!