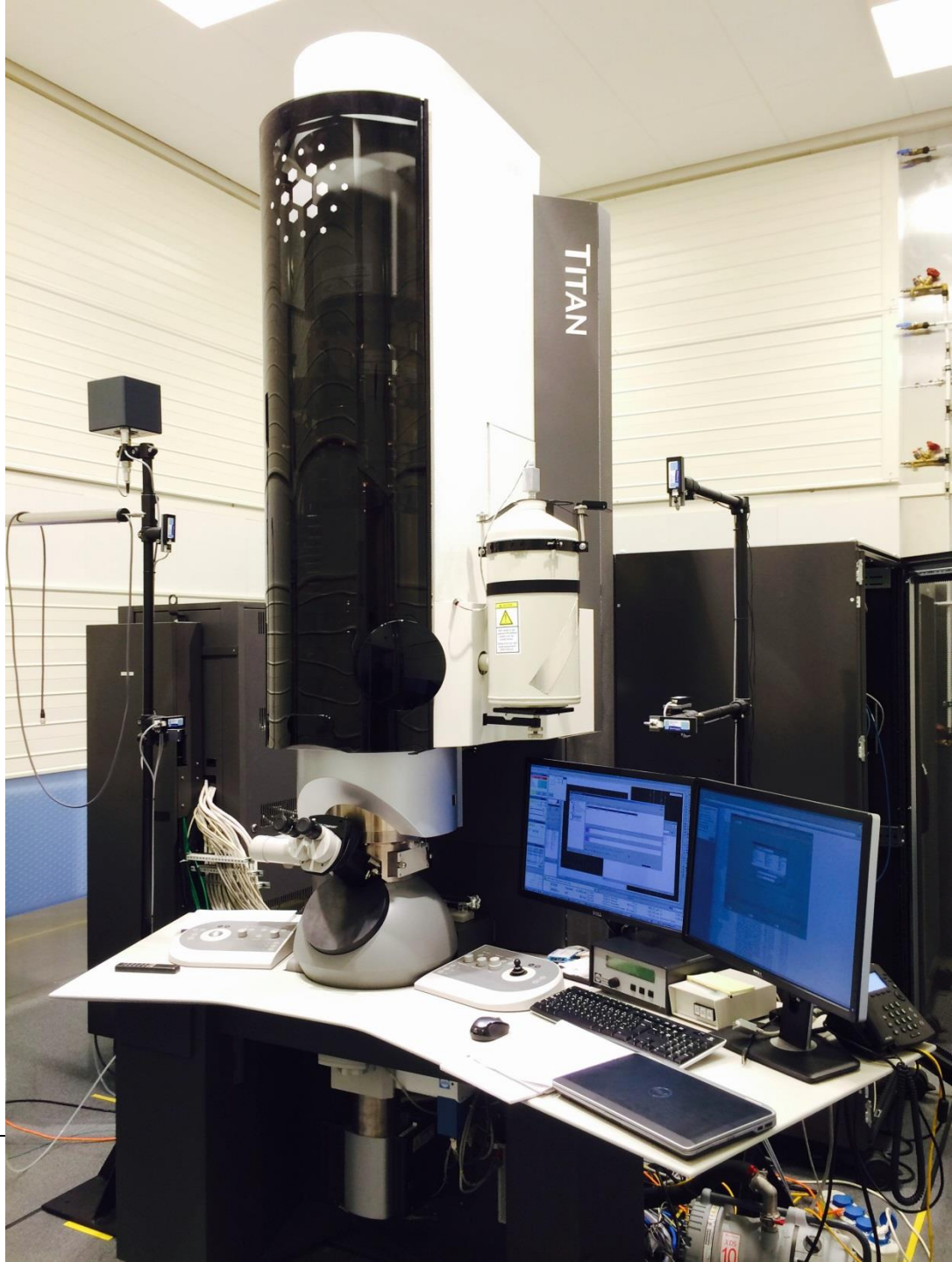
FYS 4340/FYS 9340

Diffraction Methods & Electron Microscopy

Lecture 11

CONTRAST TRANSFER FUNCTION in HRTEM



Sandeep Gorantla

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Resolution in HRTEM

Resolution of an Imaging system

Two independent origins

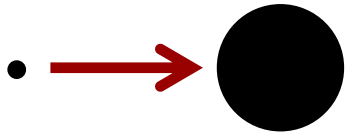
(A)Diffraction limit –

(Inherent nature of bending of light/electron waves when passes through an aperture/lens of finite size)

(B) Aberrations in the image forming lens –

(Inherent nature of the lens used in the imaging system)

EFFECT of the both (A) and (B) combined?



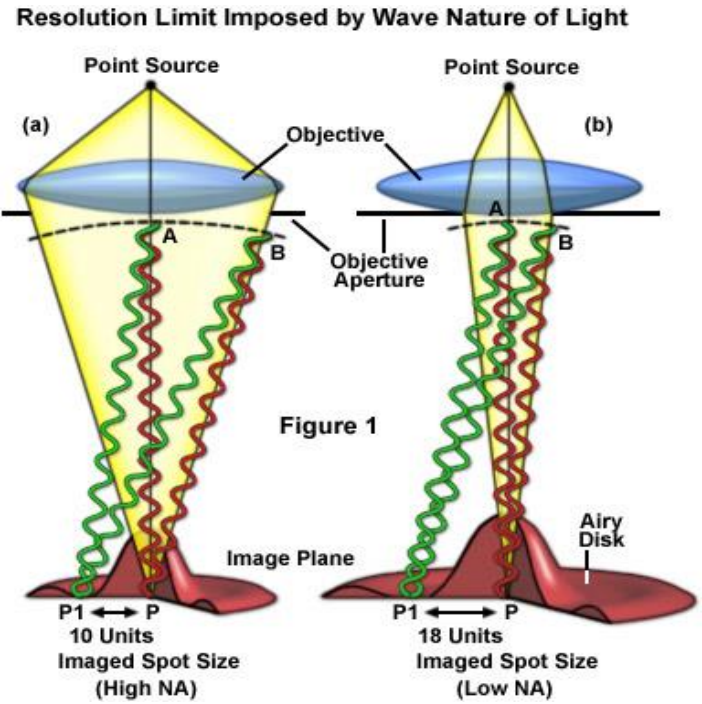
Point in object → Disc/spread out point in the image

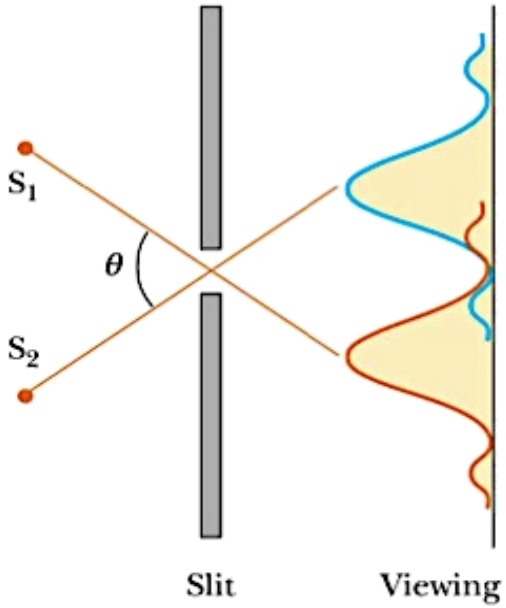
(A) Diffraction limit

Resolution of an optical system

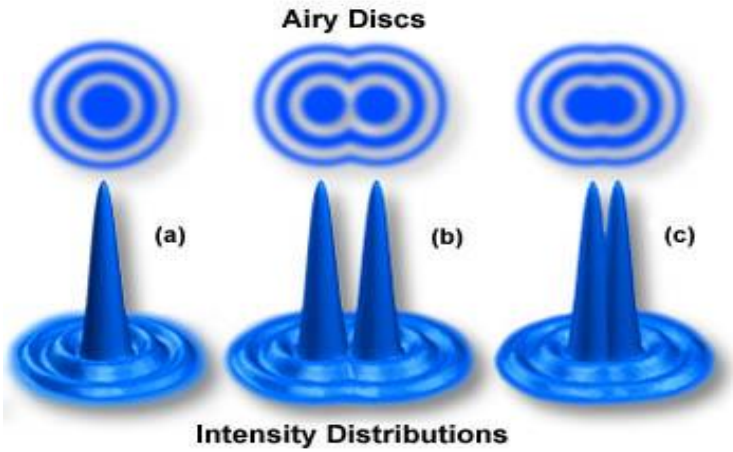
Rayleigh criterion

- The resolving power of an optical system is limited by the diffraction occurring at the optical path every time there is an aperture/diaphragm/lens.
- The aperture causes interference of the radiation (the path difference between the green waves results in destructive interference while the path difference between the red waves results in constructive interference).
- An object such as point will be imaged as a disk surrounded by rings.
- The image of a point source is called the **Point Spread Function**





Point spread function (real space)



Resolution of an optical system

Diffraction at an aperture or lens - Rayleigh criterion

The Rayleigh criterion for the resolution of an optical system states that two points will be resolvable if the maximum of the intensity of the Airy ring from one of them coincides with the first minimum intensity of the Airy ring of the other. This implies that the resolution, d_0 (strictly speaking, the resolving power) is given by:

$$d_o = 0.61 \cdot \frac{\lambda}{\eta \cdot \mathrm{Sin}(\alpha)}$$

where λ is the wavelength, η the refractive index and α is the semi-angle at the specimen.

$\eta \cdot \mathrm{Sin}(\alpha)$ = NA (Numerical Aperture).

This expression can be derived using a reasoning similar to what was described for diffraction gratings (path differences…).

When d_0 is small the resolution is high!

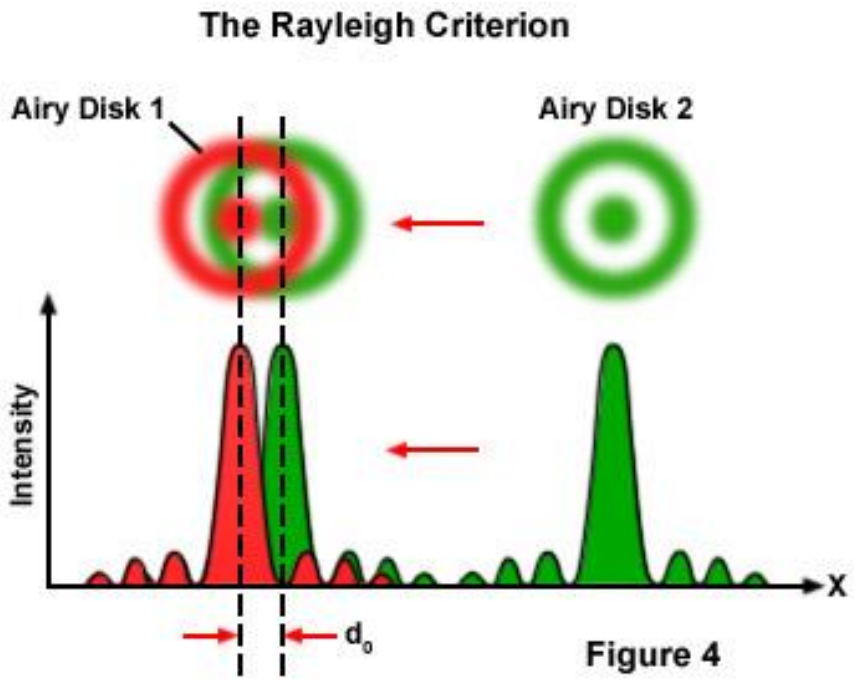
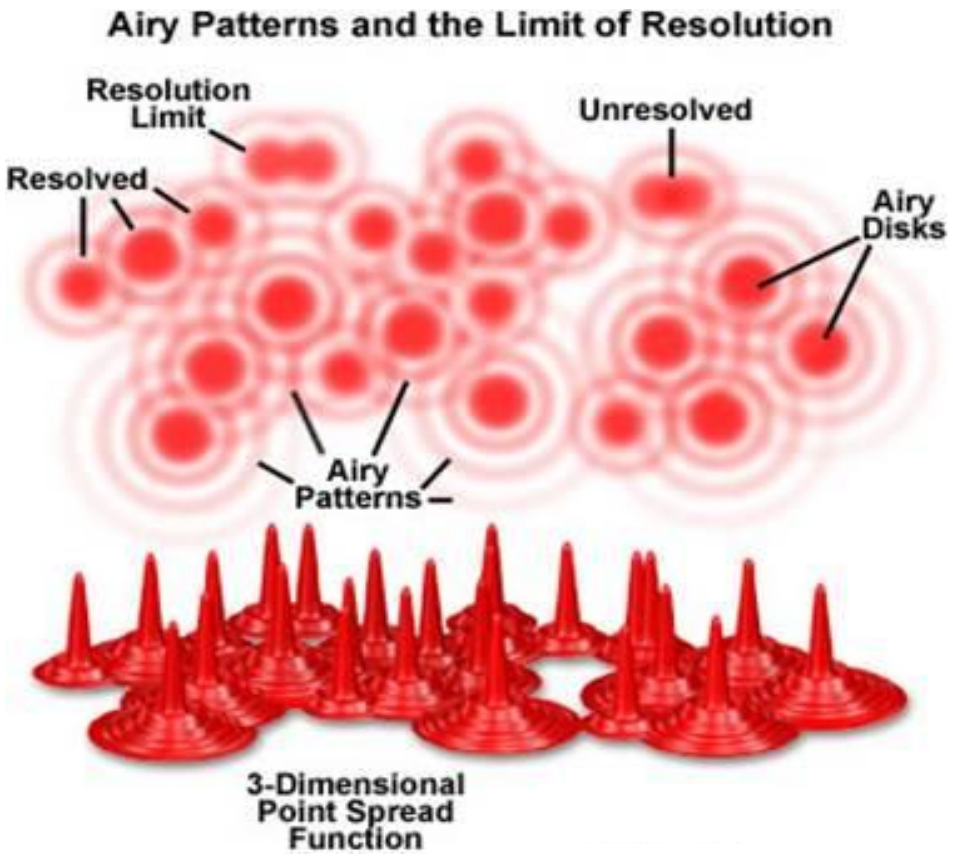


Figure 4

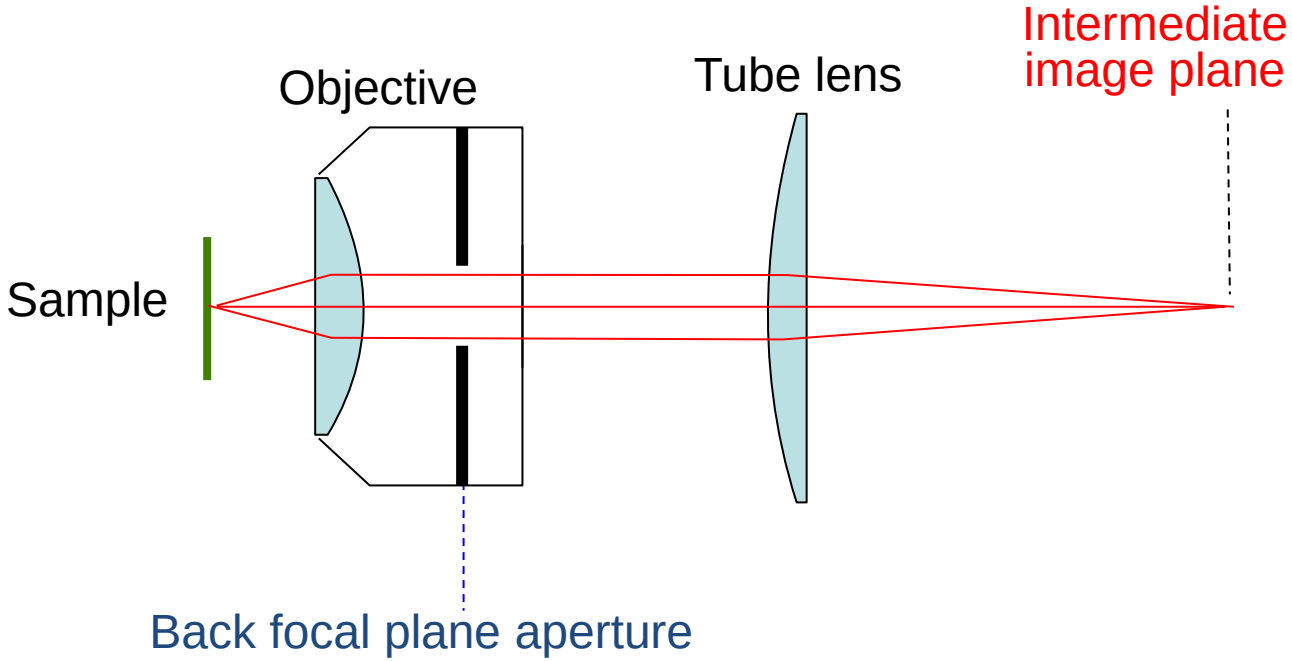
Resolution of an optical system

http://micro.magnet.fsu.edu/primer

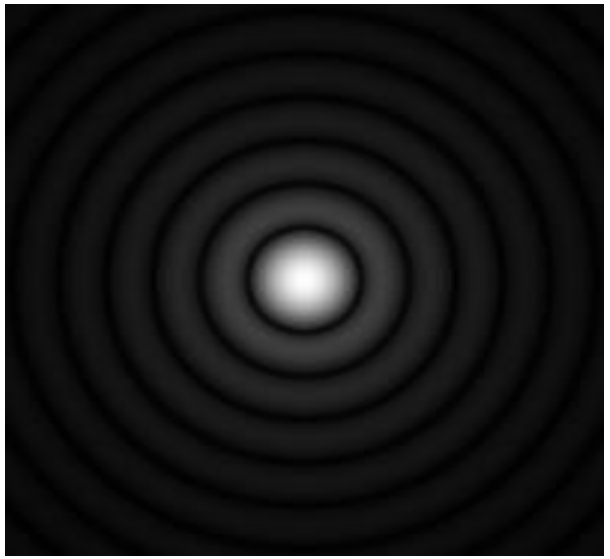
Diffraction at an aperture or lens – Image resolution



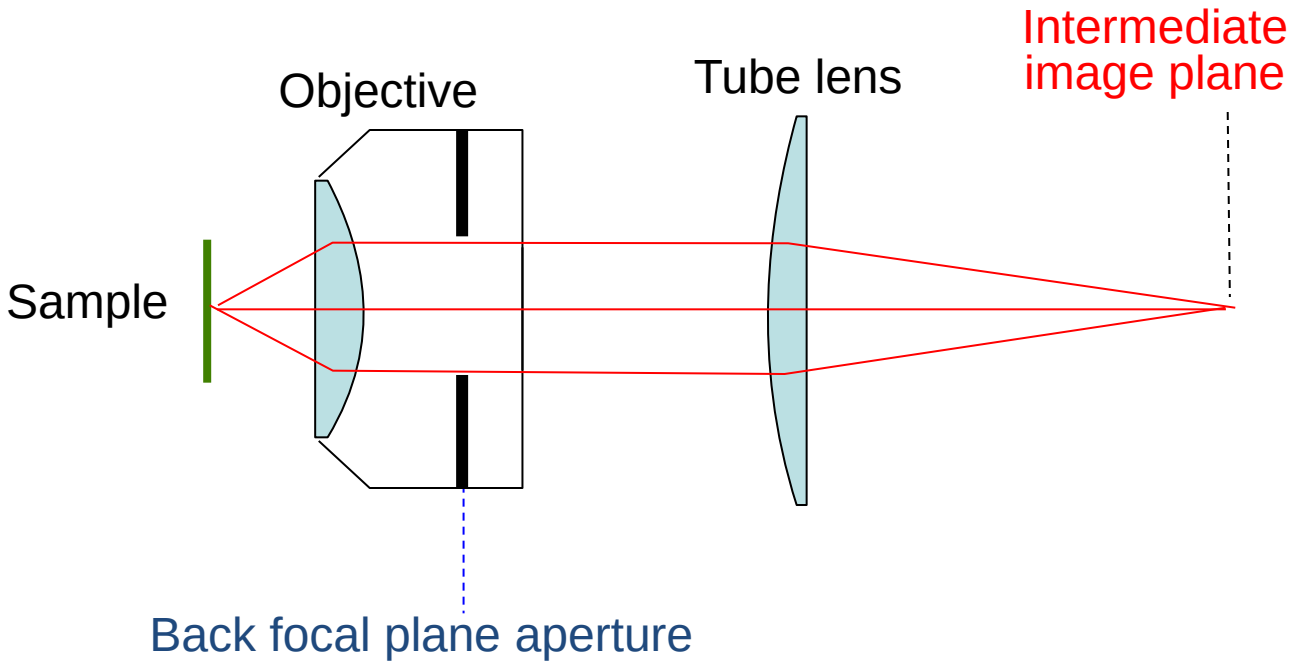
Aperture and resolution of an optical system



Diffraction spot
on image plane
= ***Point Spread Function***



Aperture and resolution of an optical system



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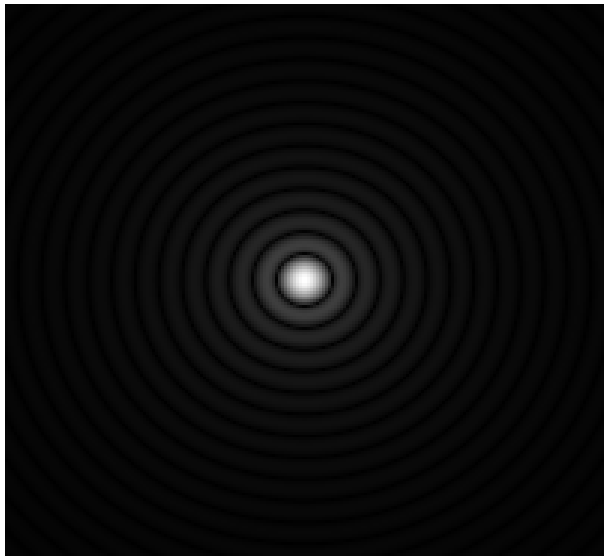
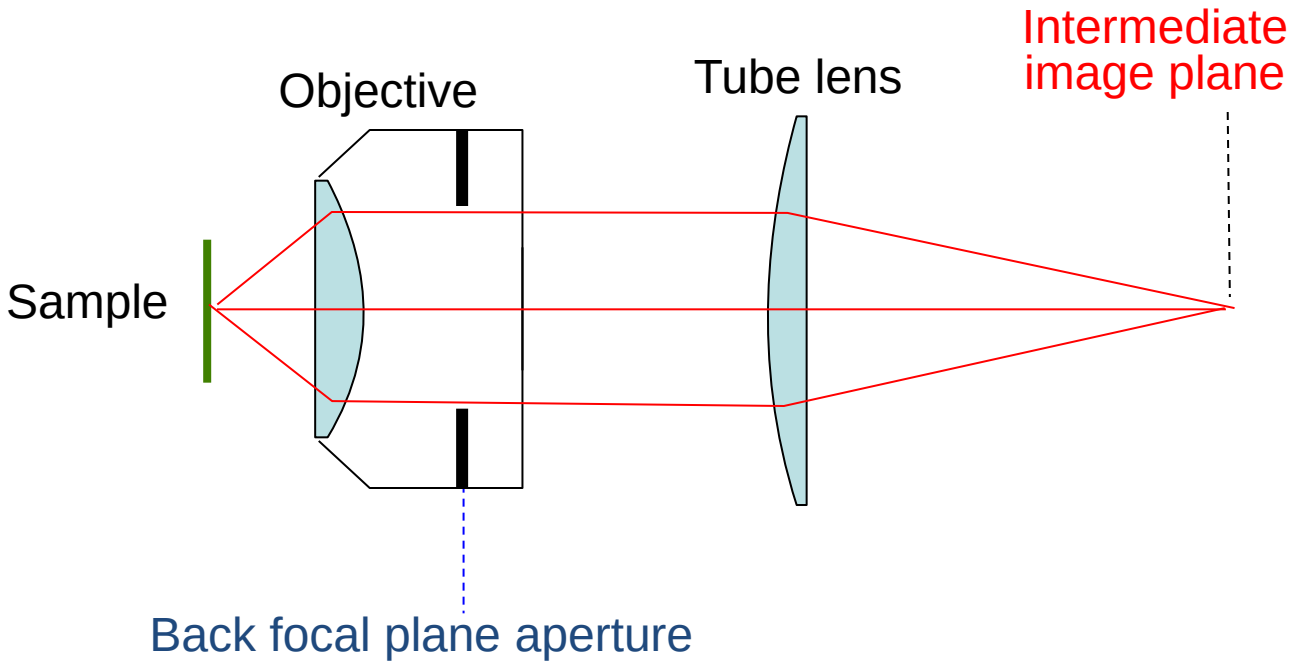


Aperture and resolution of an optical system



Diffraction spot
on image plane
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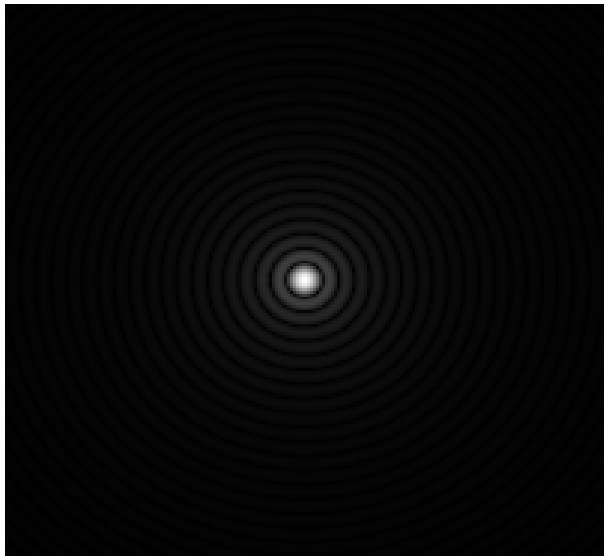
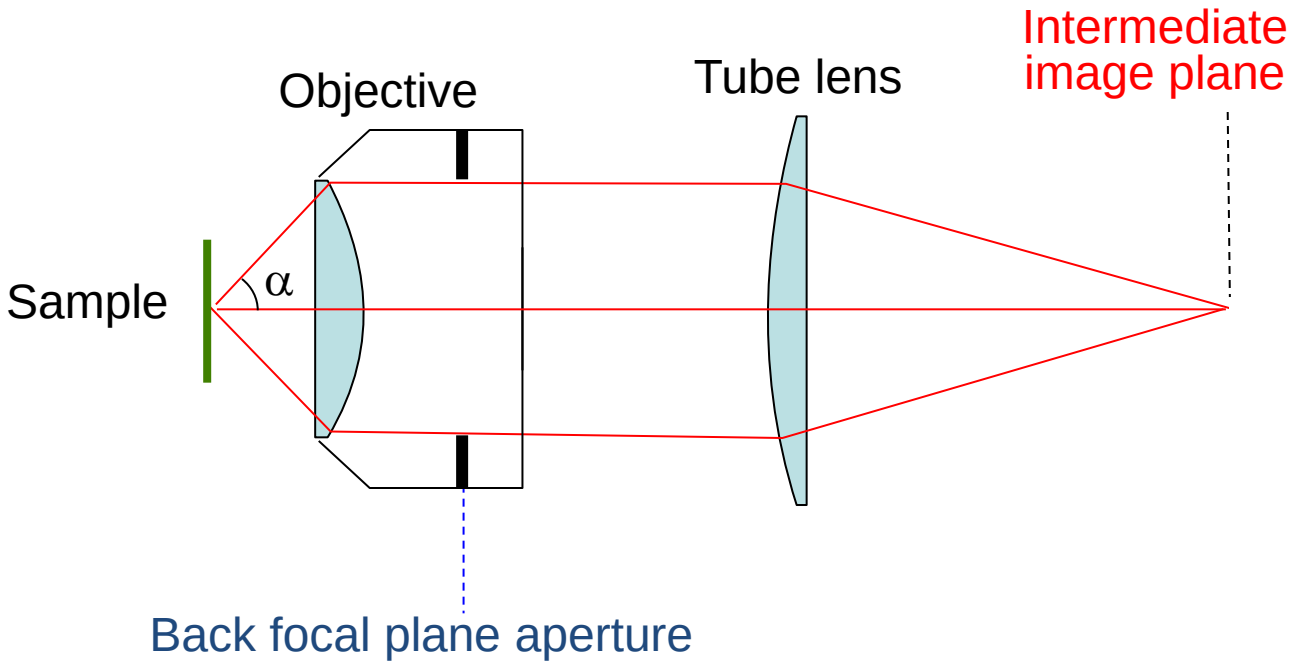
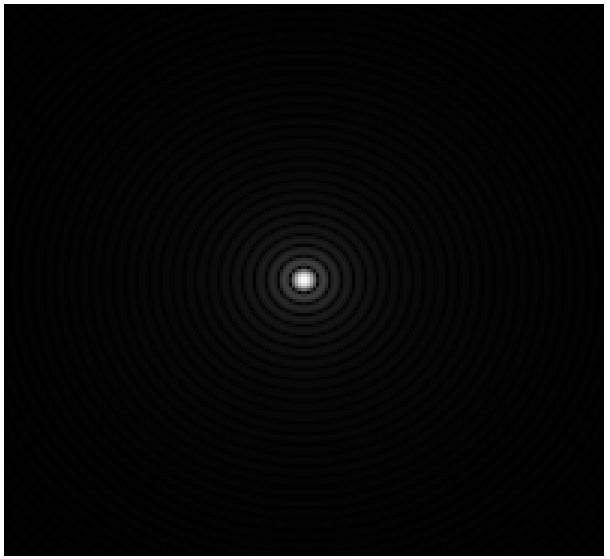


Aperture and resolution of an optical system

Diffraction spot
on image plane
= ***Point Spread Function***





The larger the aperture at the back focal plane (diffraction plane), the larger α and higher the resolution (smaller disc in image plane)

$NA = n \sin(\alpha)$

where: α = light gathering angle
n = refractive index of medium

Resolution of an Imaging system

Two independent origins

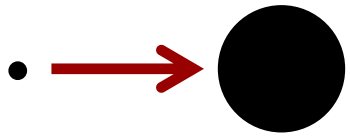
(A)Diffraction limit –

(Inherent nature of bending of light/electron waves when passes through an aperture/lens of finite size)

(B) Aberrations in the image forming lens –

(Inherent nature of the lens used in the imaging system)

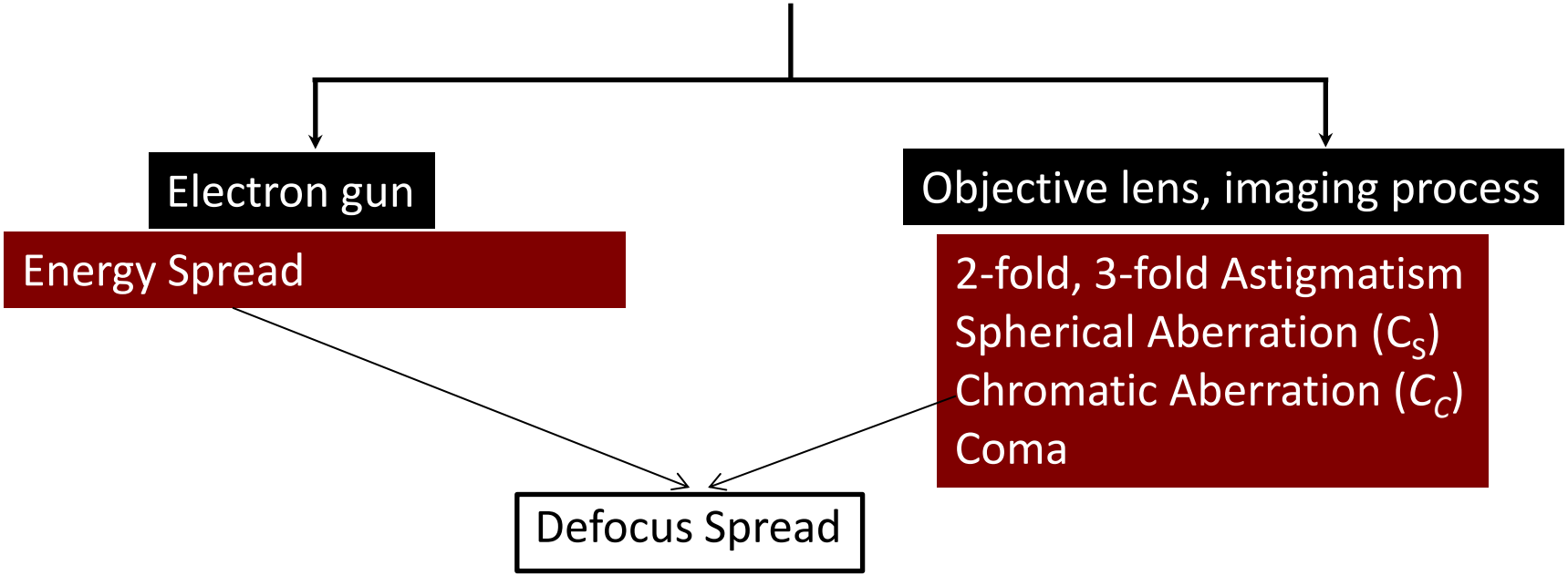
EFFECT of the above?



Point in object → Disc/spread out point in the image

(B) Aberrations in the electro magnetic lens

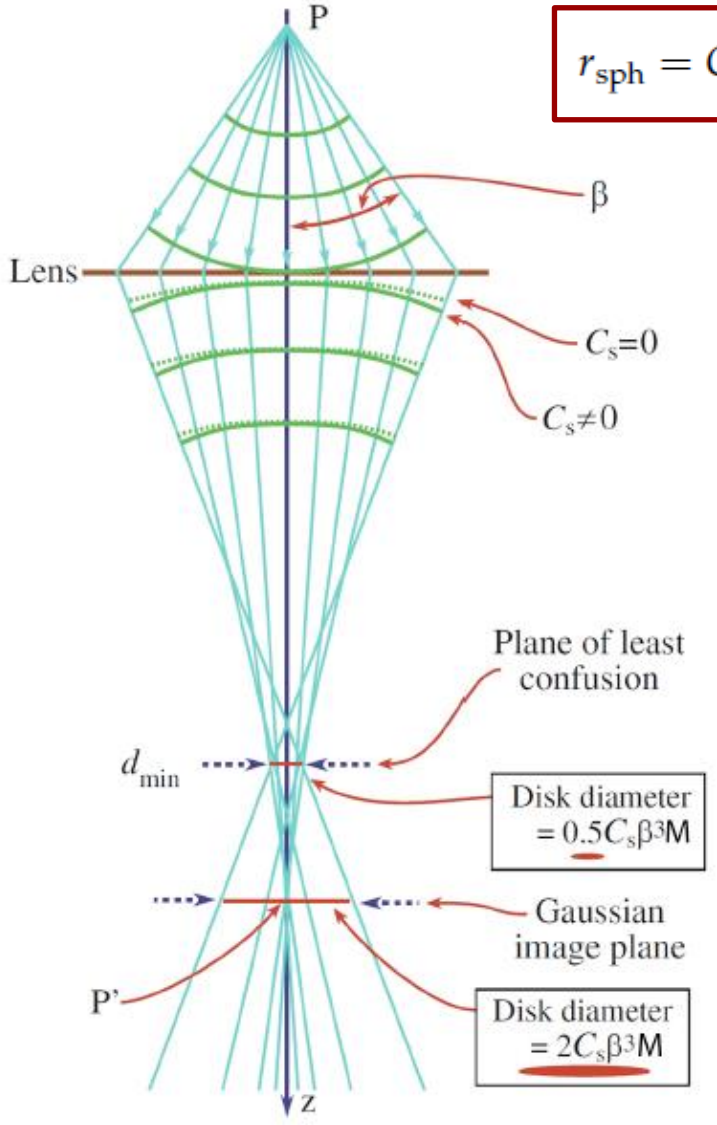
Aberrations in TEM lens



In reality, there are atleast about 10 different kinds of lens aberrations in TEM lenses that impose limitation of final resolution!!!

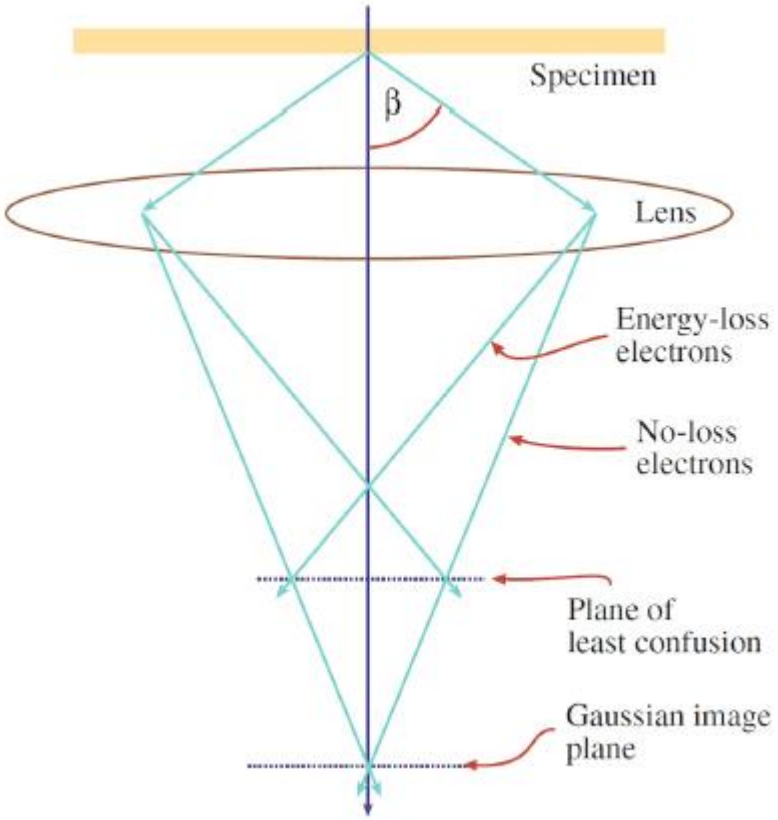
Spherical aberration coefficient (C_s)

$$r_{sph} = C_s \beta^3 M$$



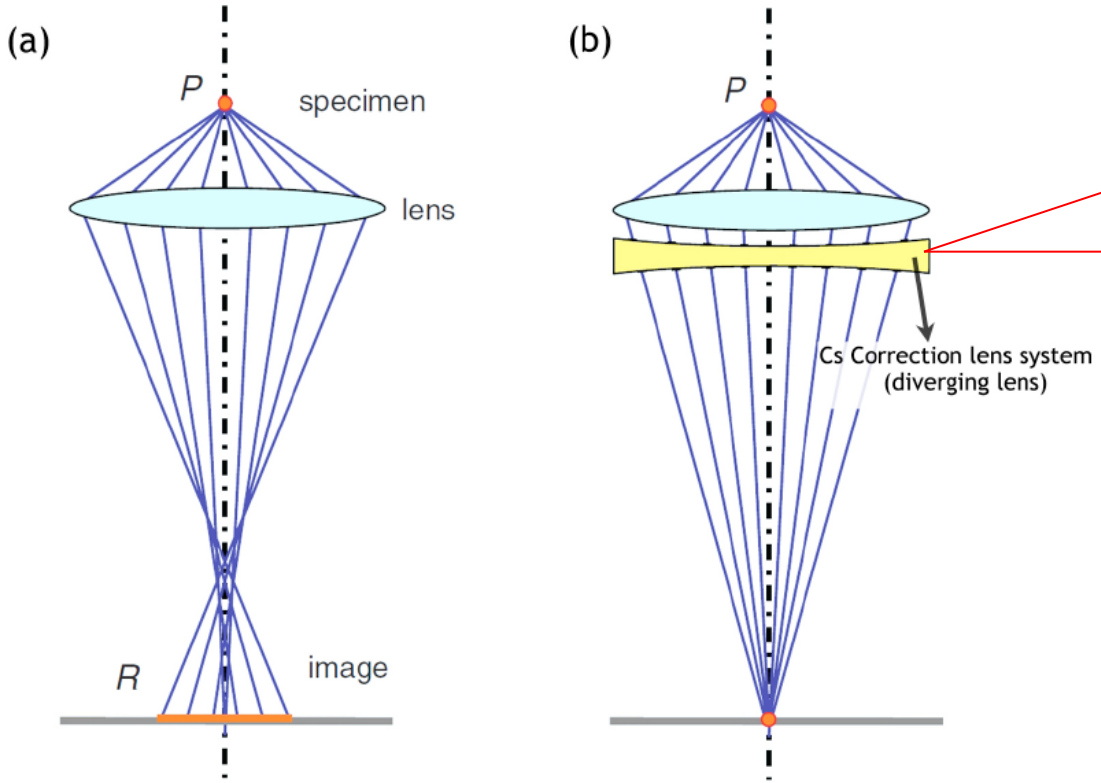
Chromatic aberration coefficient (C_c)

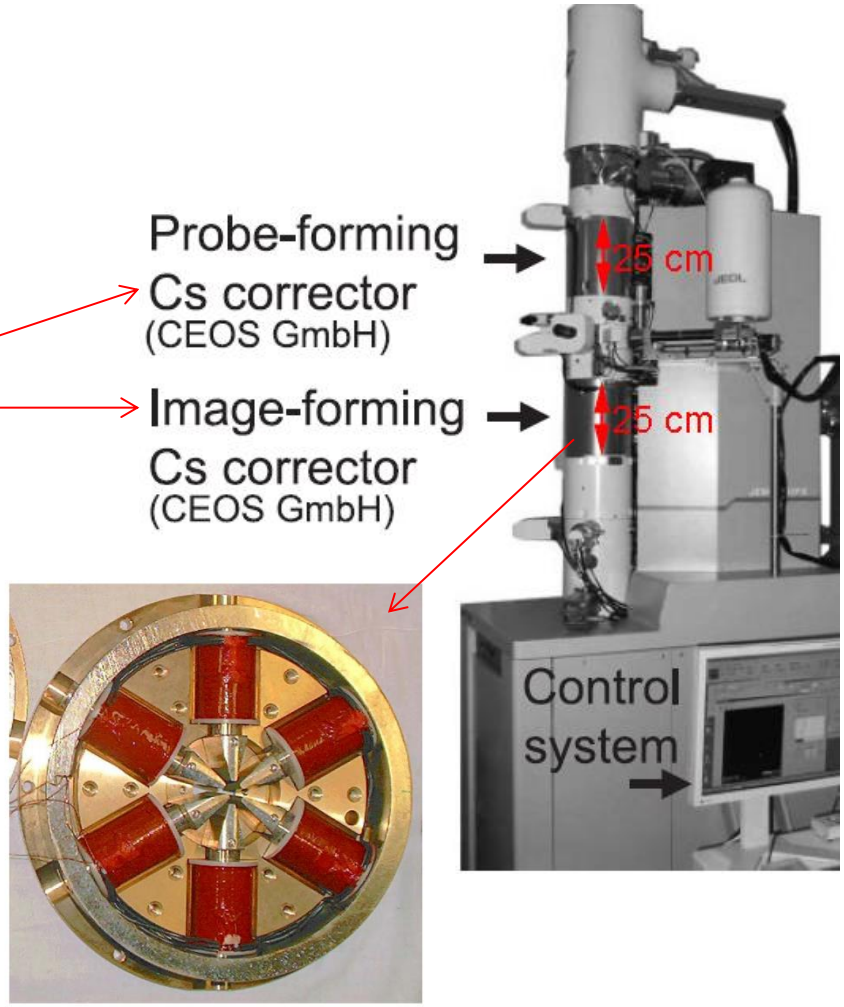
$$r_{chr} = C_c \cdot \left[\left(\frac{\Delta E}{E_0}\right)^2 + 2\left(\frac{\Delta I}{I}\right)^2 \right]^{\frac{-1}{2}} \beta M$$



TEM Lens Aberrations

Schematic of spherical aberration correction





Courtesy: Knut W. Urban, Science 321, 506, 2008; CEOS gmbh, Germany; www.globalsino.com

Resolution of an Imaging system

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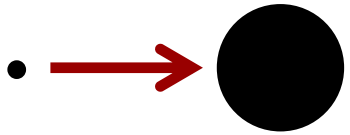


Point in object → Disc/spread out point in the image

How can we now describe the effect of point spread function of an imaging system mathematically???

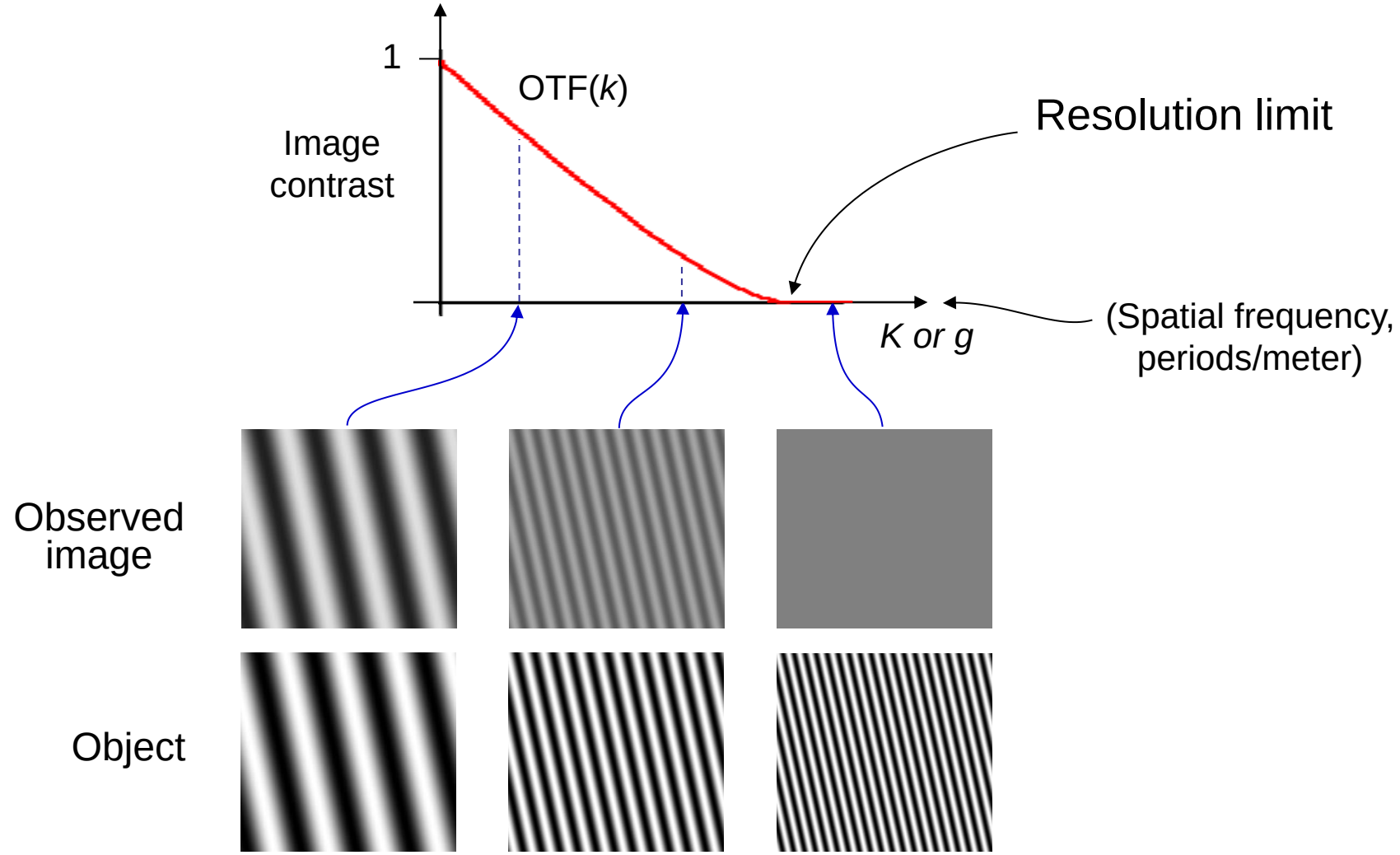
FOURIER TRANSFORMATIONS (FT)

FT of PSF in light Microscope **= OTF (Optical Transfer Function)**

FT of obj. lens image formation in HRTEM **= CTF (Contrast Transfer Function)**

New concept:
Contrast Transfer Function (CTF)

Optical Transfer Function (OTF)



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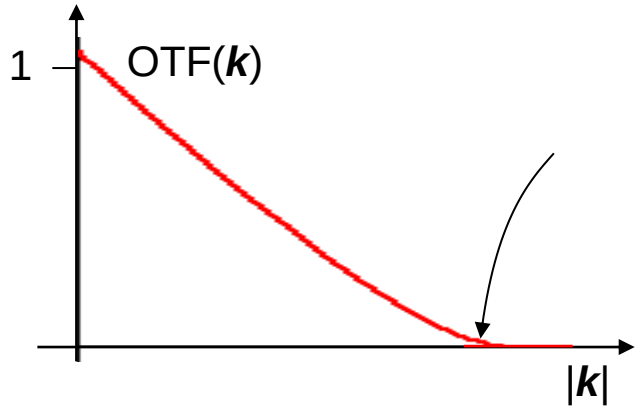
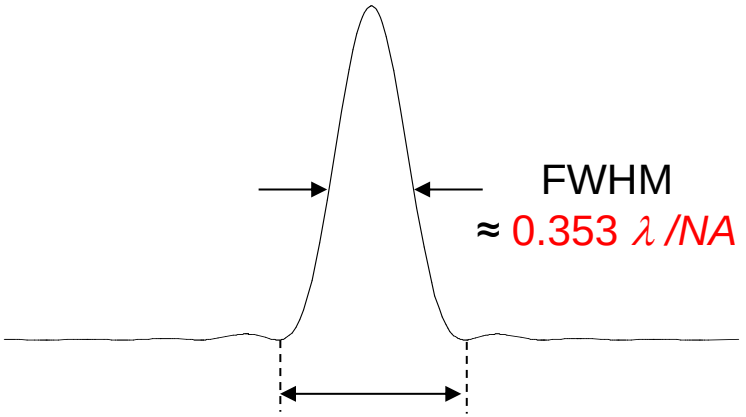
Definitions of Resolution

As the OTF cutoff frequency



$1/k_{max}$
$= 0.5\ \lambda /NA$

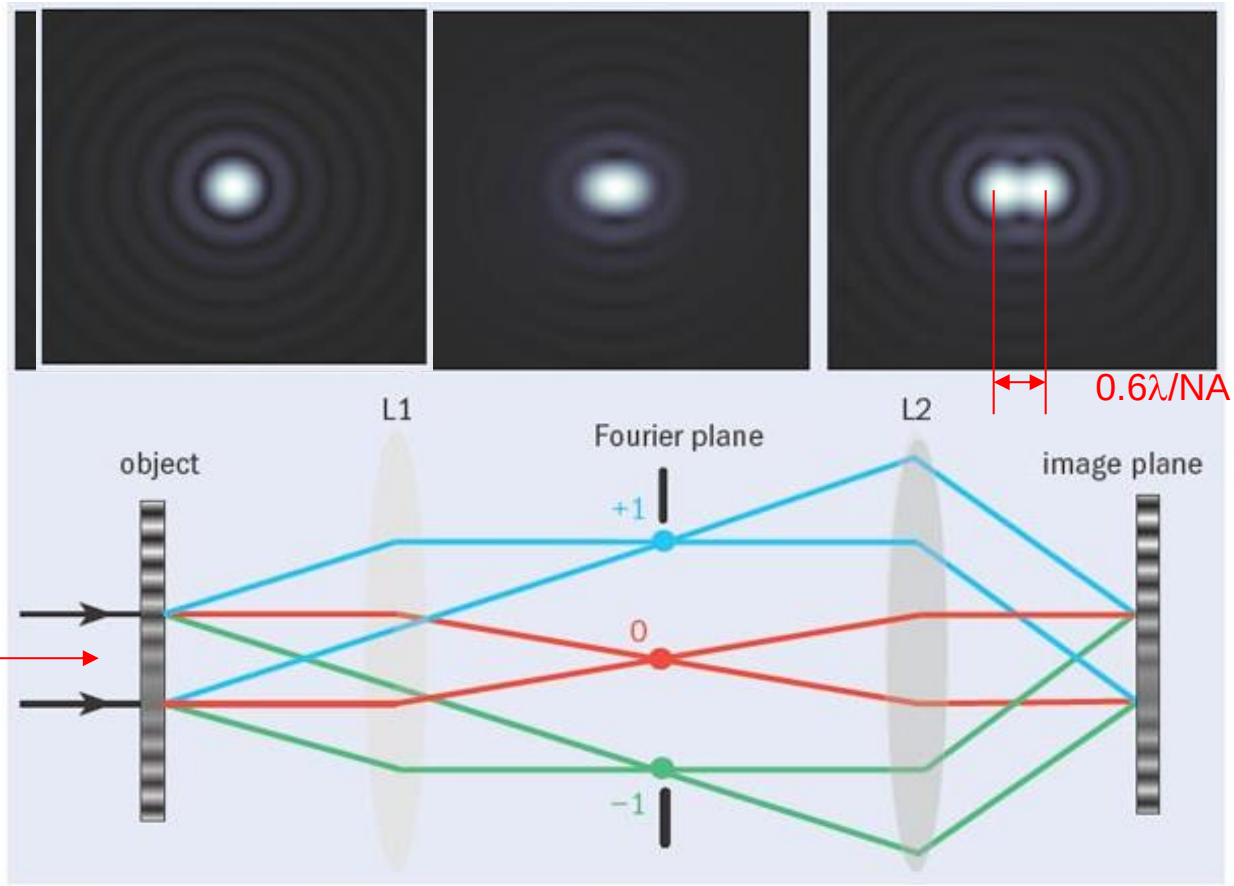
As the Full Width at Half Max (FWHM) of the PSF



As the diameter of the Airy disk (first dark ring of the PSF) = “Rayleigh criterion”

Airy disk diameter
$\approx 0.61\ \lambda /NA$

Resolution Criteria



Rayleigh's description

Abbe's description

Aberration free systems

images can be considered sums of waves

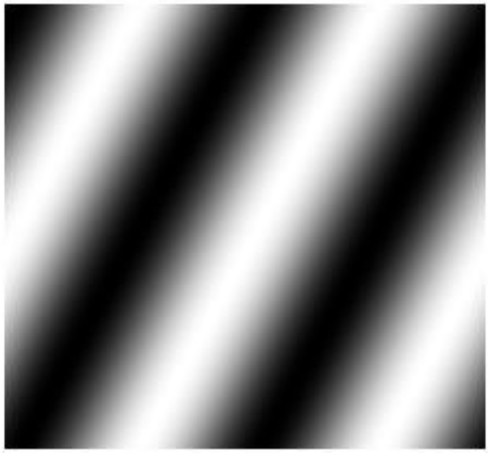
… or “spatial frequency components”

one wave

another wave

(2 waves)

+



=

(25 waves)

(10000 waves)

+ (…) =

+ (…) =

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reciprocal/frequency space

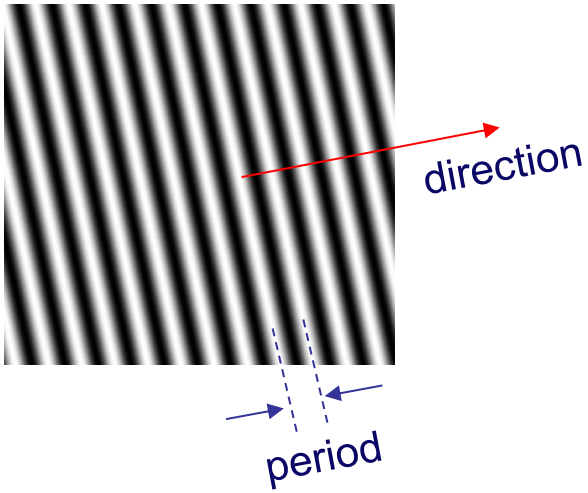
To ***describe*** a wave, specify:

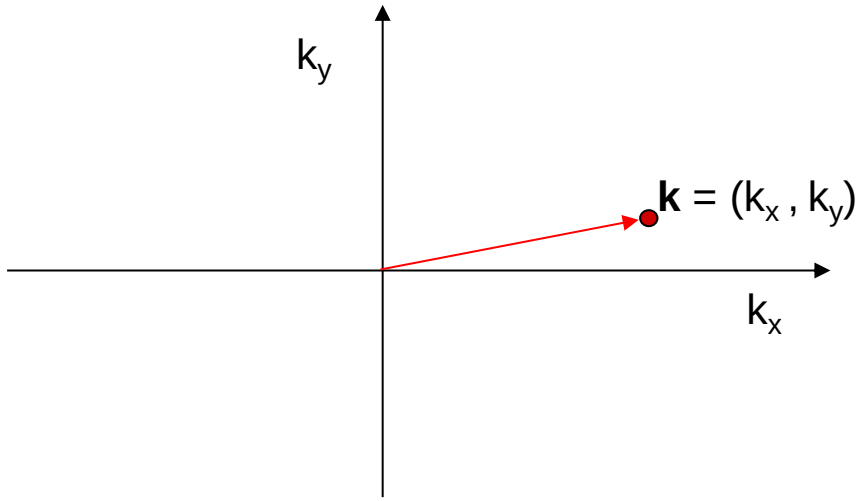
- Frequency (how many periods/meter?)
- Direction
- Amplitude (how strong is it?)
- Phase (where are the peaks & troughs?)

A wave can also be described by a complex number at a *point:*

- Distance from origin
- Direction from origin
- Magnitude of value at the point
- Phase of number

complex





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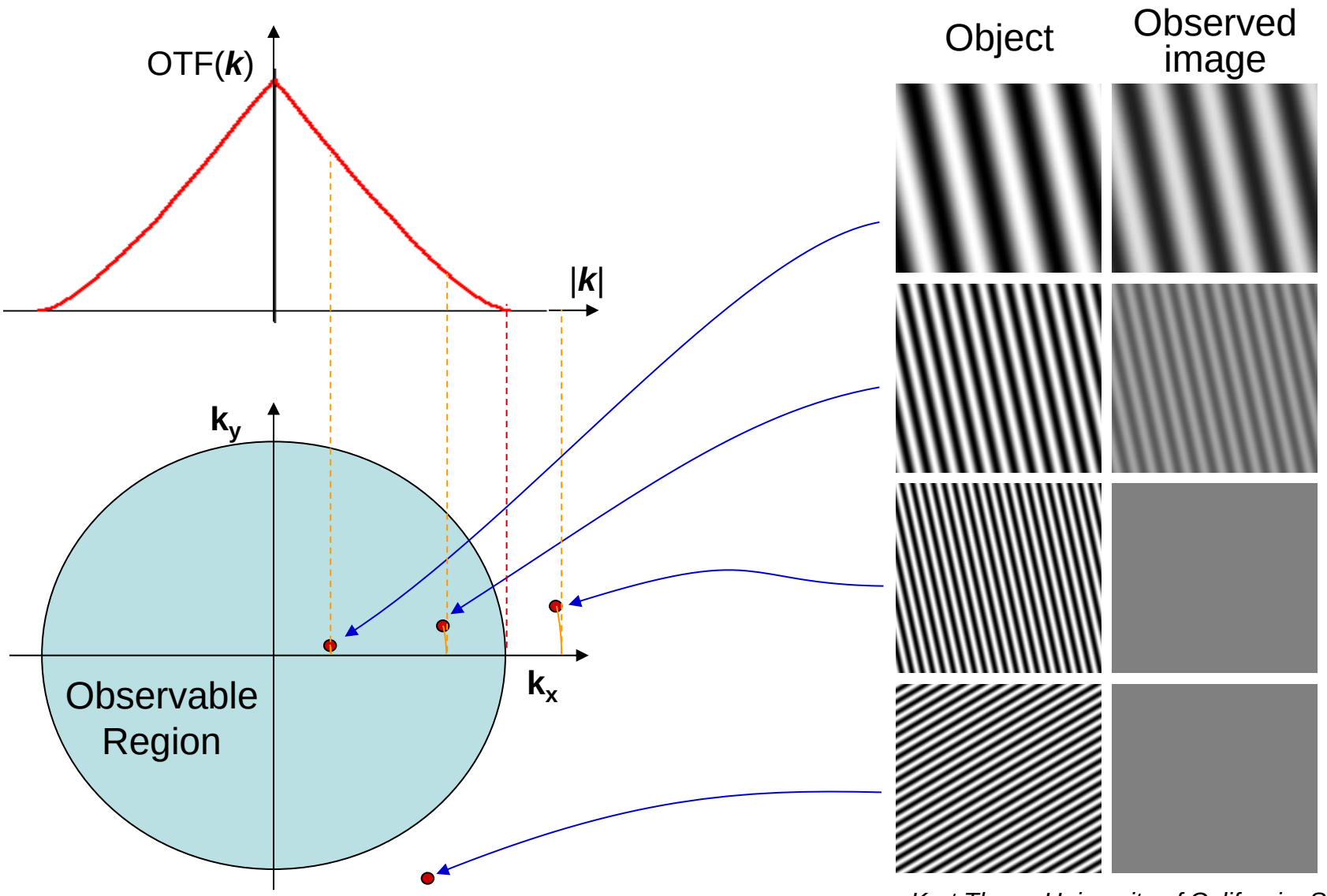
The Transfer Function Lives in Frequency Space



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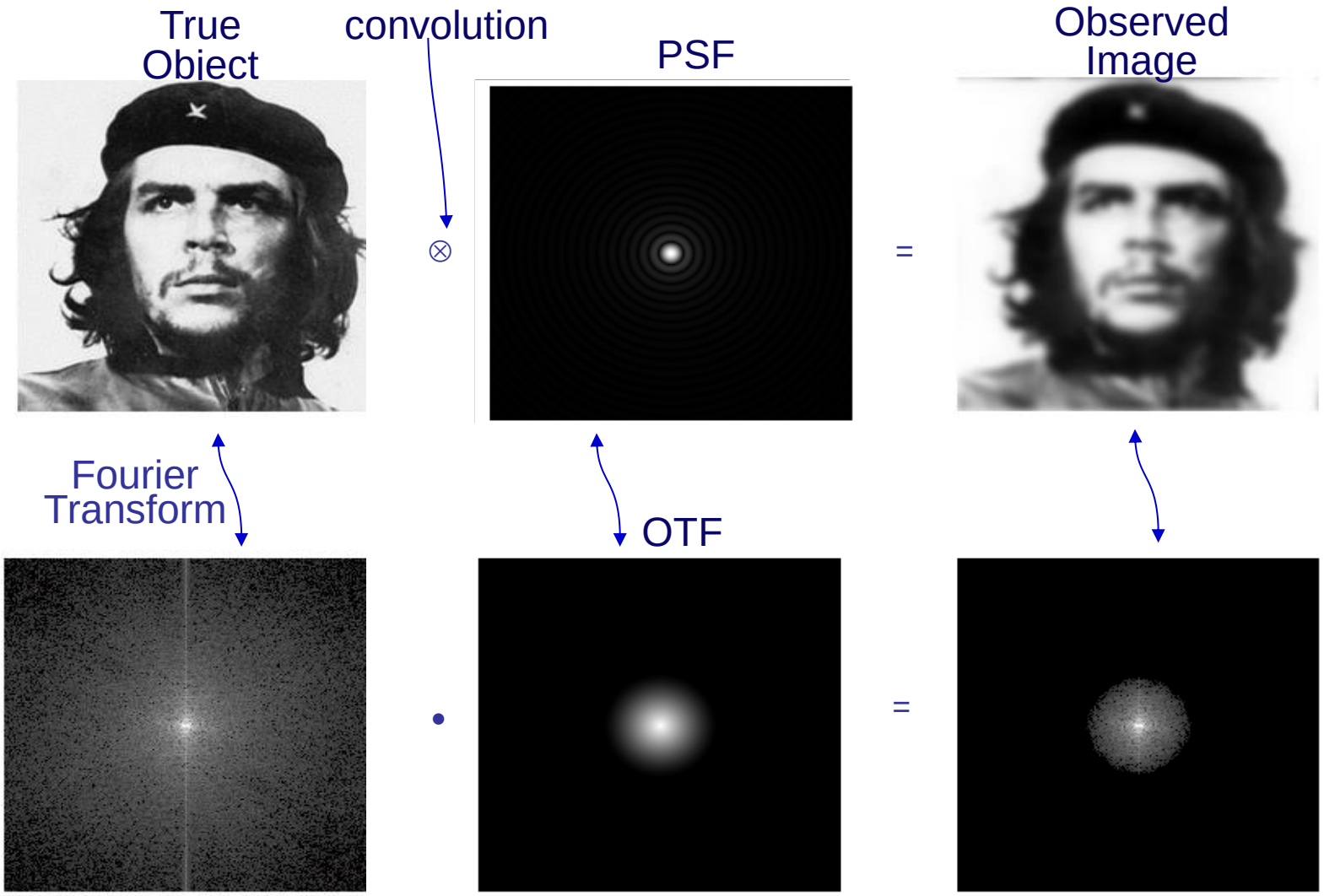
The OTF and Imaging



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Nomenclature

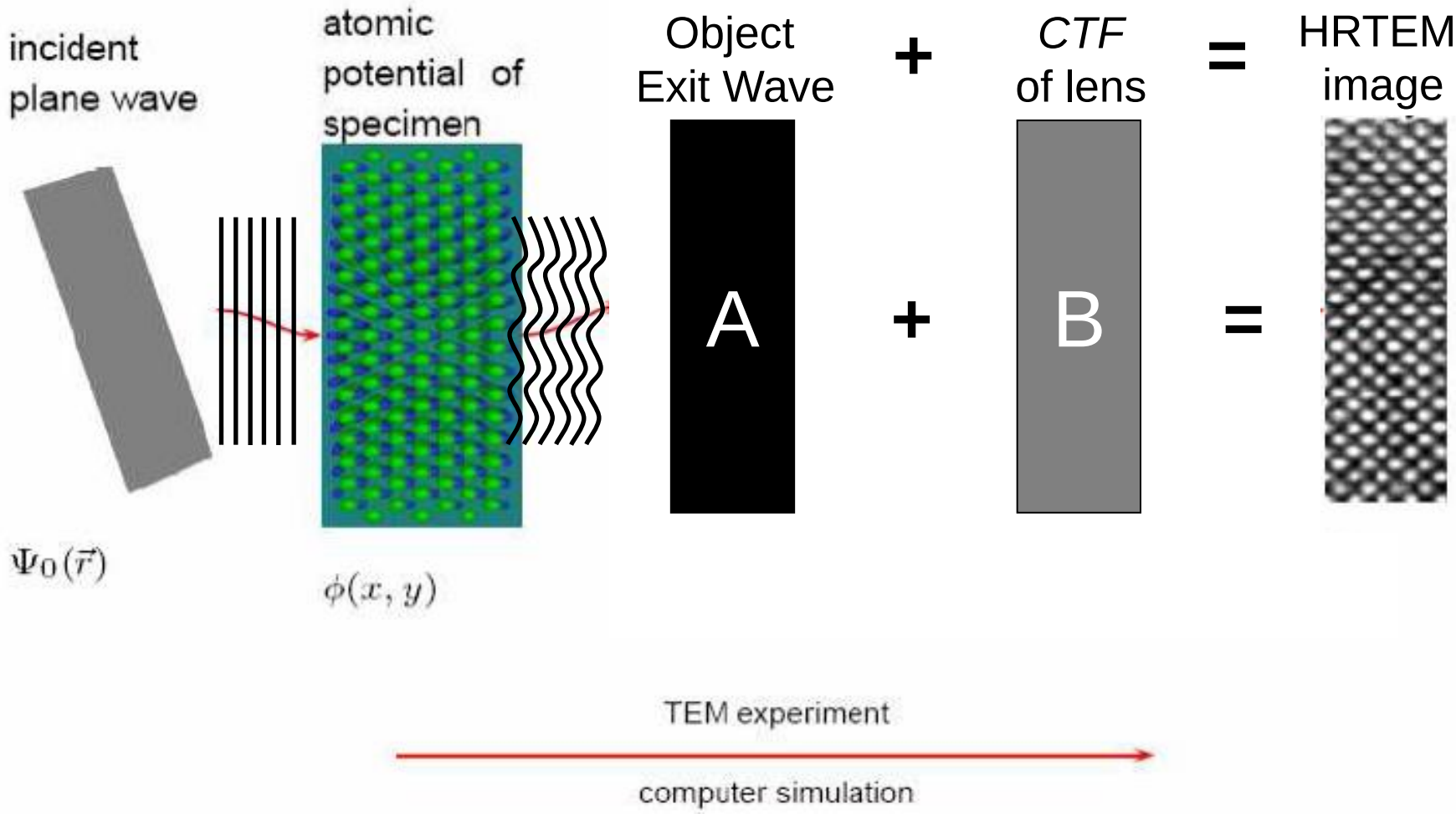
Optical transfer function, OTF
Wave transfer function, WTF
Contrast transfer function, CTF

Similar concepts:
Complex values (amplitude and phase)

Weak-phase object
very thin sample: no absorption (no change in amplitude) and only weak phase shifts induced in the scattered beams

Contrast Transfer Function in HRTEM, CTF
For weak-phase objects only the phase is considered

Principle of HRTEM formation



Courtesy: Reinhardt Otto, *Humbolt Universität Berlin.*

Principle of HRTEM formation

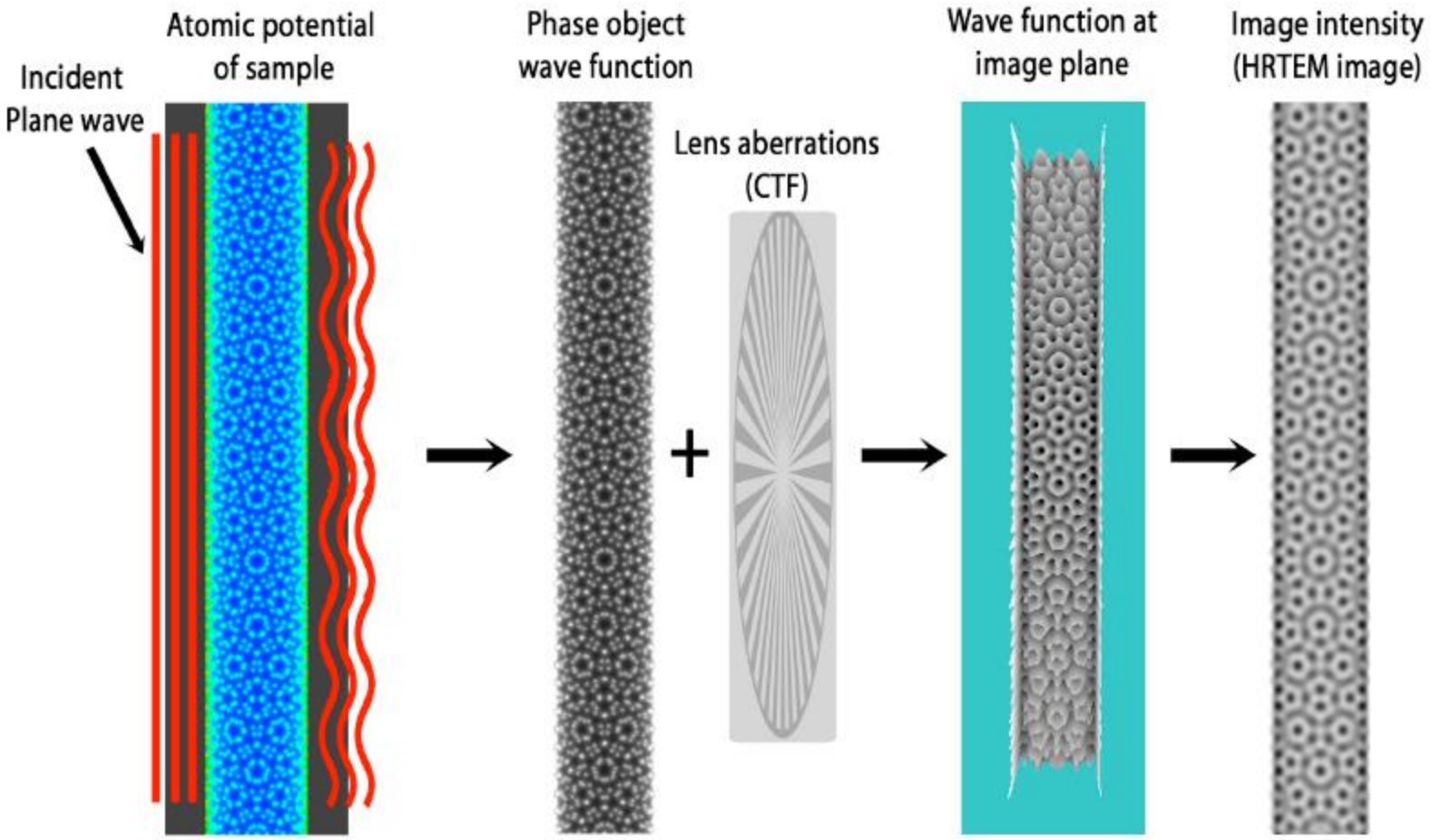


Figure 3.6: Schematic of HRTEM image formation of an individual SWCNT. It also represents the principle of HRTEM image simulation process.

Resolution in HRTEM

In optical microscopy, it is possible to define point resolution as the ability to resolve individual point objects. This resolution can be expressed (using the criterion of Rayleigh) as a quantity independent of the nature of the object.

The resolution of an electron microscope is more complex. Image "resolution" is a measure of the spatial frequencies transferred from the image amplitude spectrum (exit-surface wave-function) into the image intensity spectrum (the Fourier transform of the image intensity). This transfer is affected by several factors:

- the phases of the diffracted beams exiting the sample surface,
- additional phase changes imposed by the objective lens defocus and spherical aberration,
- the physical objective aperture,
- coherence effects that can be characterized by the microscope spread-of-focus and incident beam convergence.

For thicker crystals, the frequency-damping action of the coherence effects is complex but for a thin crystal, i.e., one behaving as a weak-phase object (WPO), the damping action can best be described by quasi-coherent imaging theory in terms of envelope functions imposed on the usual phase-contrast transfer function.

The concept of HRTEM resolution is only meaningful for thin objects and, furthermore, one has to distinguish between **point resolution** and **information limit**.

O'Keefe, M.A., Ultramicroscopy, 47 (1992) 282-297

Contrast transfer function

In the Fraunhofer approximation to image formation, the intensity in the back focal plane of the objective lens is simply the Fourier transform of the wave function exiting the specimen. Inverse transformation in the back focal plane leads to the image in the image plane.

If the phase-object approximation holds (no absorption), the image of the specimen by a perfect lens shows no amplitude modulation. In reality, a combination with the extra phase shifts induced by defocus and the spherical aberration of the objective lens generates suitable contrast.

The influence of these extra phase shifts can be taken into account by multiplying the wavefunction at the back focal plane with functions describing each specific effect. The phase factor used to describe the shifts introduced by defocus and spherical aberration is:

$$\chi(q)=\pi\lambda\Delta f q^2 + 1/2\pi Cs\lambda^3 q^4$$

with Δf the defocus value and Cs the spherical aberration coefficient. The function that multiplies the exit wave is then:

$$B(q) = \exp(i\chi(q))$$

If the specimen behaves as a weak-phase object, only the imaginary part of this function contributes to the contrast in the image, and one can set:

$$\boldsymbol{B(q) = 2\sin(\chi(q))}$$

The phase information from the specimen is converted into intensity information by the phase shift introduced by the objective lens and this equation determines the weight of each scattered beam transferred to the image intensity spectrum. **For this reason, sin(χ) is known as the contrast transfer function (CTF) of the objective lens or Phase Contrast Transfer Function.**

WEAK PHASE OBJECT APPROXIMATION

- Object very thin
- induces no amplitude modulation of the incident wave (no absorption)
- Only induces very weak phase shift on the scattered wave

Then, the contrast in the image is only due the additional phase shift on this exit scattered wave induced by Objective Lens

(a) Defocus Δf
(b) Spherical Aberration C_s

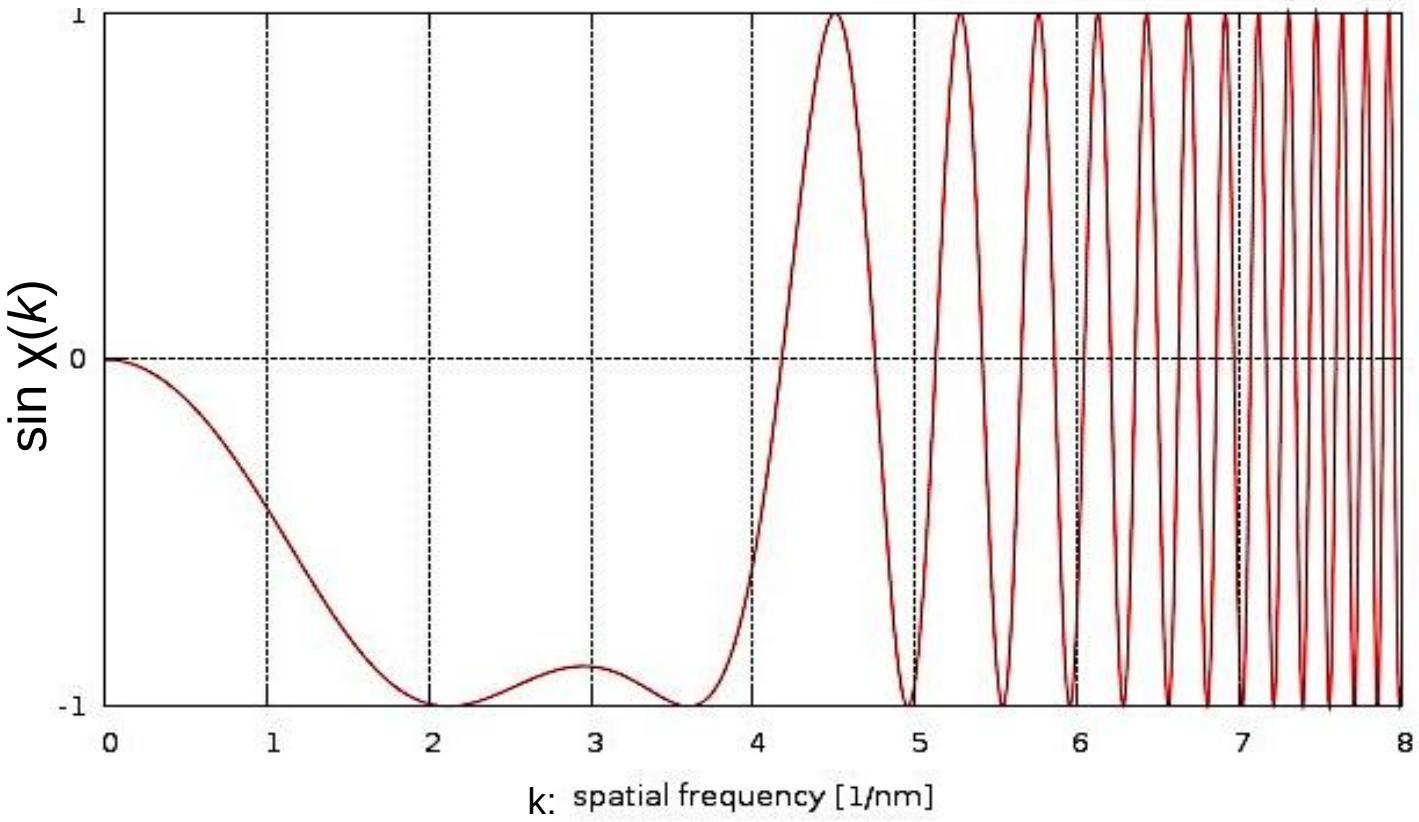
Contrast Transfer Function:

$$B(q) = \sin(\phi(q)) = \sin(\frac{1}{2}\pi\lambda^3 q^4 C_s + \pi\lambda\Delta f \cdot q^2)$$

q = Spatial Frequency (In Fourier space or Reciprocal scape), corresponding distance in image plane is 1/q

Contrast transfer function

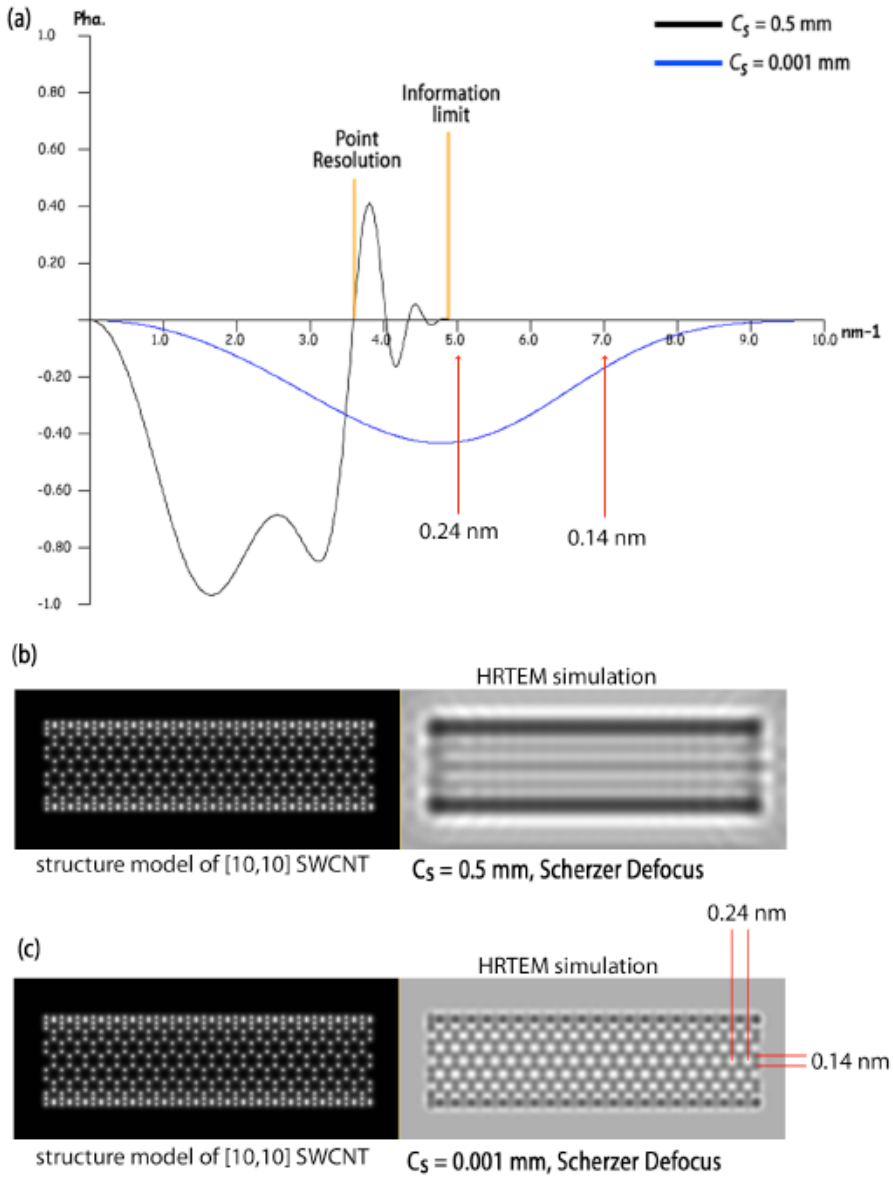
$$\sin \chi(k) = \sin(\pi\lambda\Delta f k^2 + 1/2\pi Cs\lambda^3 k^4)$$



parameters: λ=0.0025 nm (200 kV), c_s =1.1 mm, Δf= - 60 nm

The CTF oscillates between -1 (negative contrast transfer) and +1 (positive contrast transfer). The exact locations of the zero crossings (where no contrast is transferred, and information is lost) depends on the defocus.

Point resolution



Optimum defocus (Scherzer Defocus)

$$\Delta f_{sch} = -1.2 \cdot \sqrt{(C_s \lambda)}$$

$$r_{sch} = 0.66 \cdot (C_s \lambda^3)^{\frac{1}{4}}$$

Scherzer defocus

Every zero-crossing of the graph corresponds to a contrast inversion in the image.

Up to the first zero-crossing k_0 the contrast does not change its sign.

The reciprocal value $1/k_0$ is called Point Resolution.

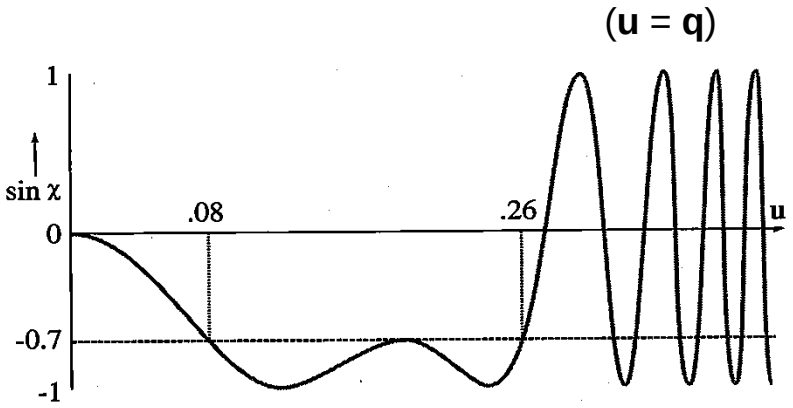
The defocus value which maximizes this point resolution is called the Scherzer defocus.

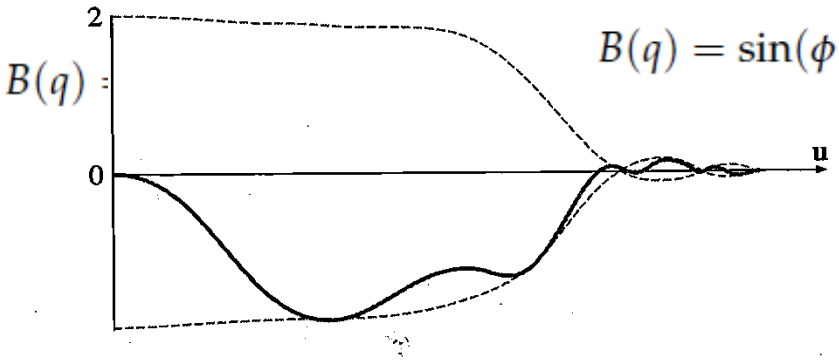
Optimum defocus: At Scherzer defocus, by choosing the right defocus value Δf one flattens $\chi(u)$ and creates a wide band where low spatial frequencies $\boldsymbol{k}$ are transferred into image intensity with a similar phase.

Working at Scherzer defocus ensures the transmission of a broad band of spatial frequencies with constant contrast and allows an unambiguous interpretation of the image.

The Envelope functions

The resolution is also limited by the spatial coherence of the source and by chromatic effects (changes of electron energy in time):





Phase Contrast Transfer Function:

For Weak Phase Object Approximation:

$$B(q) = \sin(\phi(q)) = \sin(\frac{1}{2}\pi\lambda^3 q^4 C_s - \pi\lambda\Delta f \cdot q^2)$$

Envelope Functions

$$B(q) = \sin(\phi(q)) = \sin(\frac{1}{2}\pi\lambda^3 q^4 C_s - \pi\lambda\Delta f \cdot q^2) \cdot [E_s(q) \cdot E_t(q) \cdot E_i(q) \cdot A(q)]$$

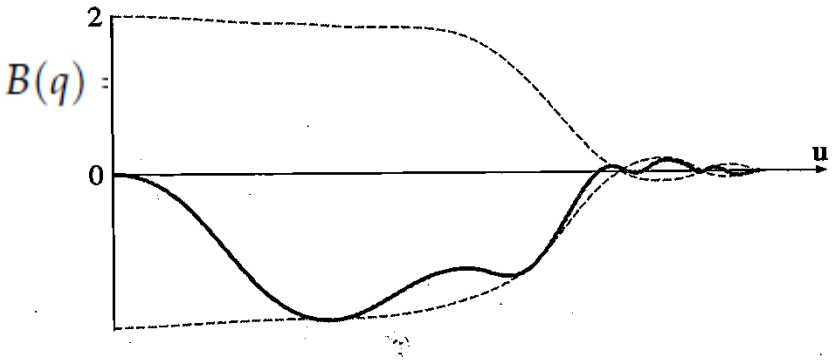
Envelope functions related to incoherencies in electron beam dampen out the CTF

The envelope function imposes a “virtual aperture” in the back focal plane of the objective lens.

The Envelope functions

$$B(q) = \sin(\phi(q)) = \sin(\frac{1}{2}\pi\lambda^3 q^4 C_s - \pi\lambda\Delta f \cdot q^2) \cdot [E_s(q) \cdot E_t(q) \cdot E_i(q) \cdot A(q)]$$

E_s and E_t represent the envelope functions of spatial and temporal coherence, E_i the instrumental instabilities and A represents the effect of objective aperture size.



E_s is *spatial coherency envelope* (caused by the finite incident beam convergence, i.e., the beam is not fully parallel)

E_t is the *temporal coherency envelope* (caused by chromatic aberrations, focal and energy spread, instabilities in the high tension and objective lens current)

Envelope functions related to incoherencies in electron beam dampen out the CTF

The envelope function imposes a “virtual aperture” in the back focal plane of the objective lens.

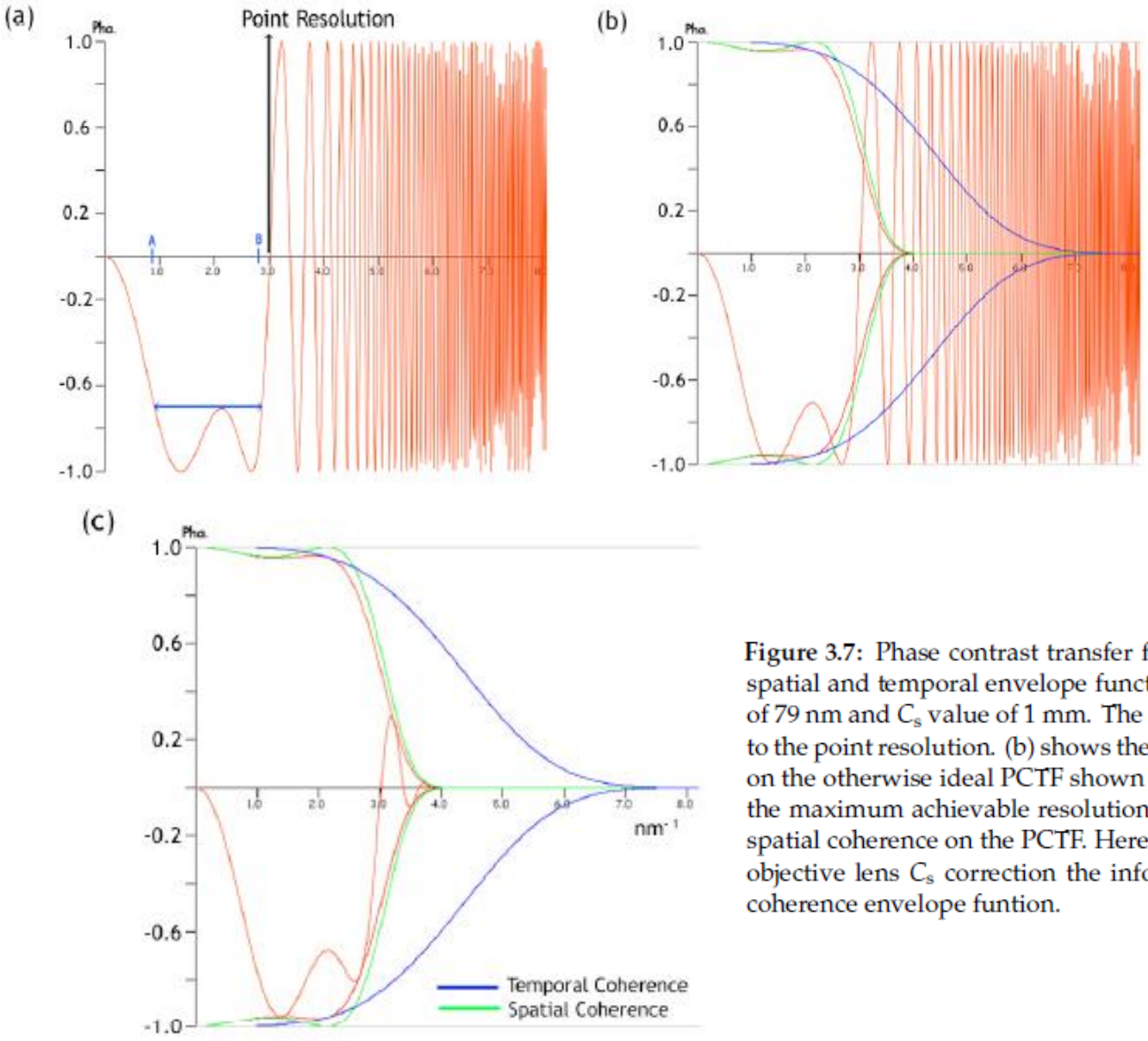


Figure 3.7: Phase contrast transfer function (PCTF). (a) The PCTF in the absence of the spatial and temporal envelope functions at 80 kV accelerating voltage, scherzer defocus of 79 nm and C_s value of 1 mm. The ordinate value of 3 nm^{-1} (i.e. ~ 0.33 nm) corresponds to the point resolution. (b) shows the overlay of spatial and temporal enevelope functions on the otherwise ideal PCTF shown in (a). (c) shows the corresponding effect of limiting the maximum achievable resolution i.e. information limiting effect of the temporal and spatial coherence on the PCTF. Here, it can be appreciated that in the absence of modern objective lens C_s correction the information limit of the TEM is limited by the spatial coherence envelope funtion.

The envelope function of spatial coherence, E_s, depends on the illumination angle of the condenser aperture (α), C_s and the defocus as given by equation 3.8. [79] This function accounts for the spatial incoherences in the electron beam emanating from the electron gun source. The lowering of C_s in aberration corrected TEMs also has the advantage of extending this spatial dampening function to higher spatial frequencies.

$$E_s(q) = \exp\left[-\frac{1}{4\ln 2}(\pi\alpha(\Delta f \cdot q + C_s\lambda^2 q^3))^2\right] \tag{3.8}$$

The temporal coherence envelope function, E_t, depends on the energy spread of the electrons at the source, chromatic aberration and the current fluctuations in the objective lens system is given by equation 3.9. [79] The temporal coherence has a more significant impact in damping the PCTF to zero i.e. in imposing the information limit of the TEM. Also, owing to effect of energy spread included in this envelope function the temporal incoherence also leads to defocus spread in the HRTEM image.

$$E_t(q) = \exp\left[-\frac{1}{16\ln 2}(\pi\lambda^2 q^2 \cdot \delta^2)^2\right] \tag{3.9}$$

Phase contrast and information limit

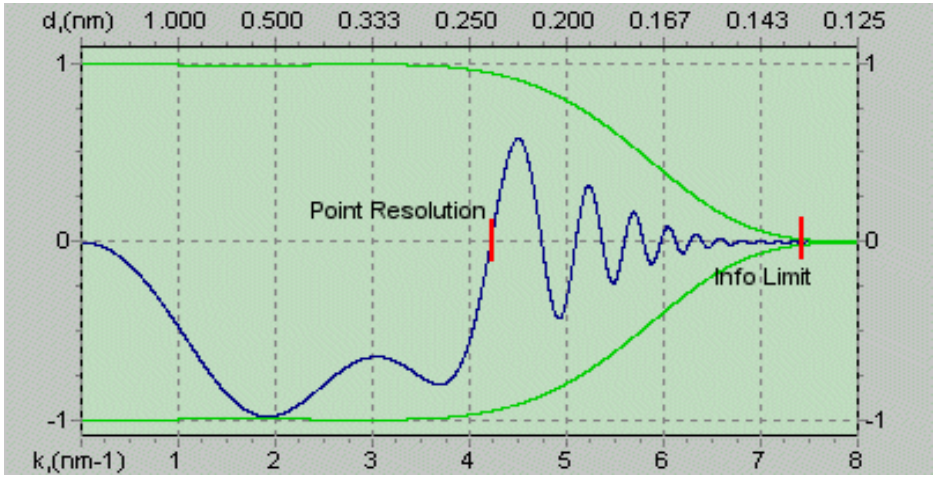
Point Resolution (or Point-to-Point, or Directly Interpretable Resolution) of a microscope corresponds to the to the point when the CTF first crosses the k-axis:

$$k = 0.67 C^{1/4} \lambda^{3/4}$$

Phase contrast images are directly interpretable only up to the point resolution (Scherzer resolution limit). If the information limit is beyond the point resolution limit, one needs to use image simulation software to interpret any detail beyond point resolution limit.

Information limit goes well beyond point resolution limit for FEG microscopes (due to high spatial and temporal coherency).

For the microscopes with thermionic electron sources (LaB6 and W), the info limit usually coincides with the point resolution.

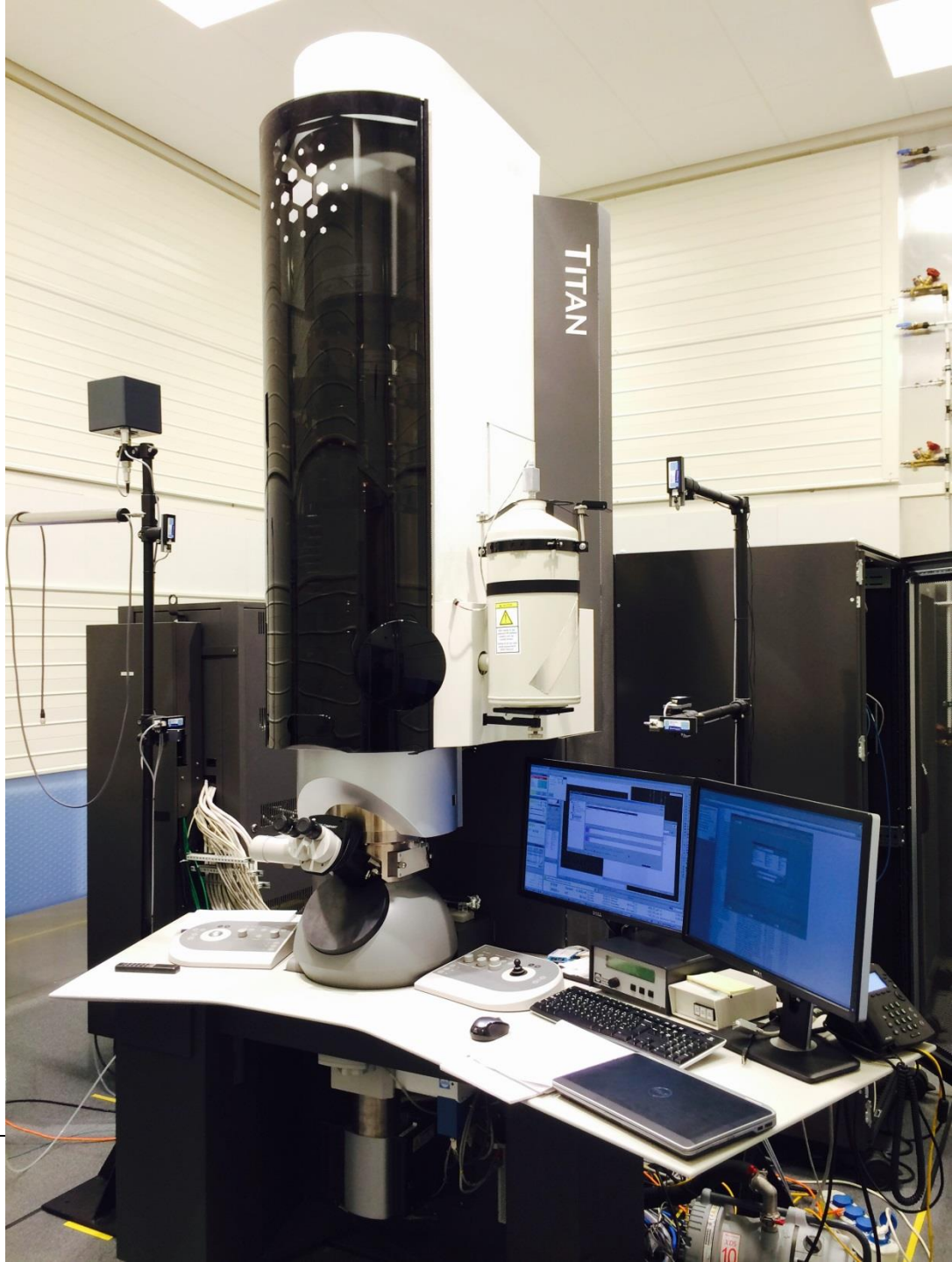


http://www.maxsidorov.com/ctfexplorer/webhelp/effect_of_defocus.htm

Important points to notice

- CTF is oscillatory: there are "passbands" where it is NOT equal to zero (good "transmittance") and there are "gaps" where it IS equal (or very close to) zero (no "transmittance").
- When it is negative, positive phase contrast occurs, meaning that atoms will appear dark on a bright background.
- When it is positive, negative phase contrast occurs, meaning that atoms will appear bright on a dark background.
- When it is equal to zero, there is no contrast (information transfer) for this spatial frequency.
- At Scherzer defocus CTF starts at 0 and decreases, then
- CTF stays almost constant and close to -1 (providing a broad band of good transmittance), then
- CTF starts to increase, and
- CTF crosses the *u*-axis, and then
- CTF repeatedly crosses the *u*-axis as *u* increases.
- CTF can continue forever but, in reality, it is modified by envelope functions and eventually dies off.

Thank you!



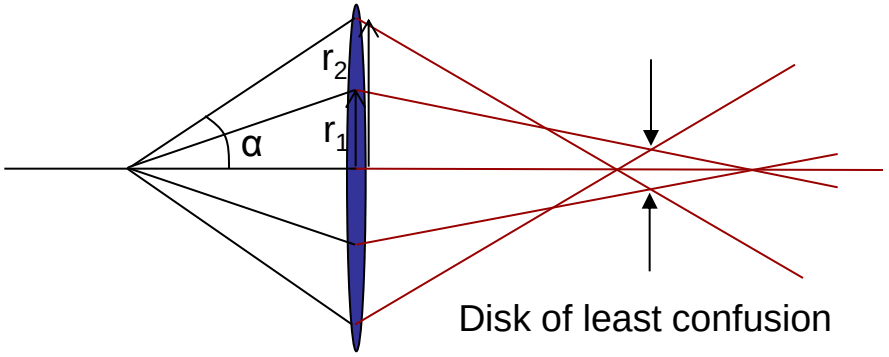
Supplementary Information

TEM Lens Aberrations

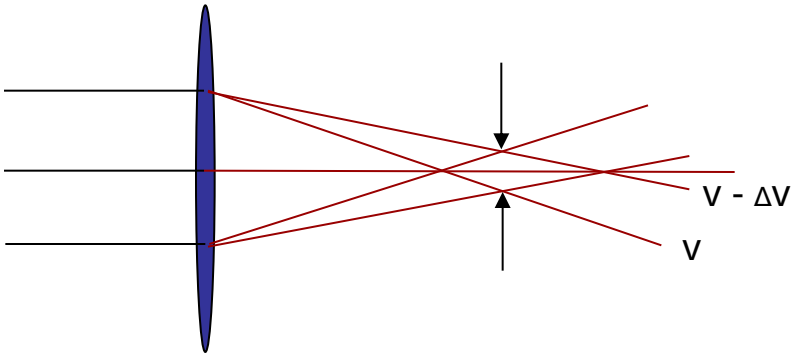
- **Spherical aberration coefficient**

  $d_s = 0.5MC_s\alpha^3$

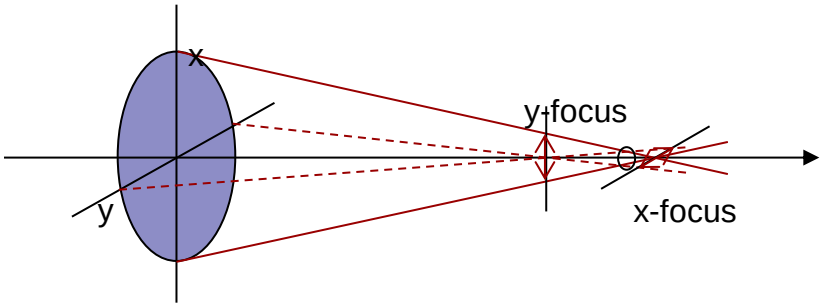
  M: magnification
  C_s :Spherical aberration coefficient
  α: angular aperture/
  angular deviation from optical axis



Spherical aberration

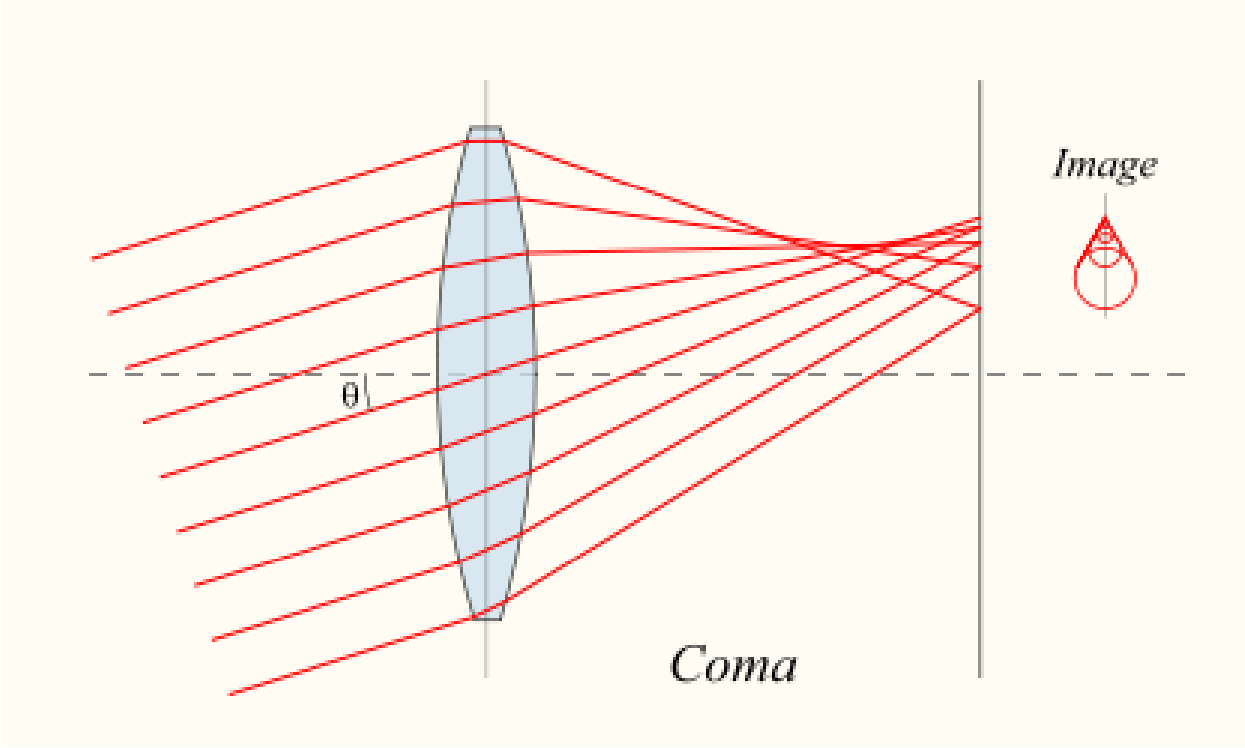


Chromatic aberration



Astigmatism

coma, or **comatic aberration**



in an optical system refers to aberration inherent to certain optical designs or due to imperfection in the lens or other components that results in off-axis point sources such as stars appearing distorted, appearing to have a tail (coma) like a comet.

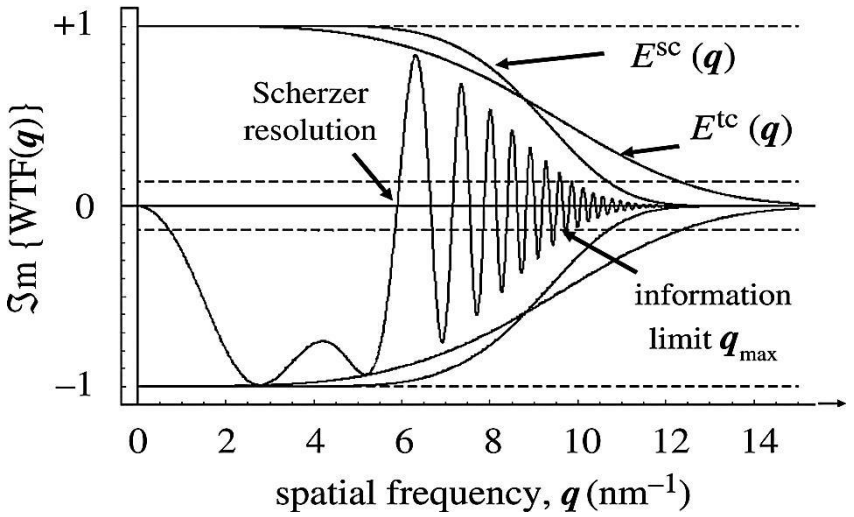
Courtesy: Wikipedia

Phase-contrast transfer function at Scherzer's defocus

The point-spread function describes the effect of the aberrations of the objective lens in real space as i.e $\mathrm{PSF}(\boldsymbol{r}) = \mathrm{FT}^{-1}[\mathrm{WTF}(\boldsymbol{q})]$, transform of the wave-transfer function defined in Fourier space w $\mathrm{WTF}(\boldsymbol{q}) = E^{\mathrm{sc}}(\boldsymbol{q}) E^{\mathrm{tc}}(\boldsymbol{q}) \exp(-\mathrm{i}\chi(\boldsymbol{q}))$,

Damping of the Fourier components is described by the envelope functions $E_{sc}(\boldsymbol{q})$ and $E_{tc}(\boldsymbol{q})$ resulting from deficiencies of spatial and temporal coherence. They damp destroy information, in particular, of the high spatial frequencies. The arising limit is called the information limit.

(***q*** = ***k***)



The imaginary part of the wave-transfer function (WTF) basically characterizes the contrast transfer from a phase-object to the image intensity. The oscillations restrict the interpretable resolution (Scherzer resolution) to below the highest spatial frequency transferred $\mathbf{q}_{max}$. $\mathbf{q}_{max}$ is called the information limit given by the envelope functions E_{sc} and E_{tc} of the restricted spatial and temporal coherence.

Lichte H et al. Phil. Trans. R. Soc. A 2009;367:3773-3793

The phase contrast transfer function PCTF, sinχ (q),

It shows the additional phase shift induced by Objective lens aberrations & defocus
on already existing phase changes in the diffracted beams after the incident electron wave has passed through specimen.

$$\chi(q) = \pi\lambda\Delta f q^2 + 1/2\pi C_s \lambda^3 q^4$$

q = Spatial Frequency (In Fourier space or Reciprocal scape), corresponding distance in image plane is 1/q

Point resolution

Point resolution: related to the finest detail that can be directly interpreted in terms of the specimen structure. Since the CTF depends very sensitively on defocus, and in general shows an oscillatory behavior as a function of *k*, the contribution of the different scattered beams to the amplitude modulation varies. However, for particular underfocus settings the instrument approaches a perfect phase contrast microscope for a range of *k* before the first crossover, where the CTF remains at values close to –1. It can then be considered that, to a first approximation, all the beams before the first crossover contribute to the contrast with the same weight, and cause image details that are directly interpretable in terms of the projected potential.

Optimisation of this behaviour through the balance of the effects of spherical aberration *vs.* defocus leads to the generally accepted *optimum defocus* $1\ -1.2(Cs\lambda)^{1/2}$. Designating an optimum resolution involves a certain degree of arbitrariness. However, the point where the CTF at optimum defocus reaches the value –0.7 for $k = 1.49C^{-1/4}\lambda^{-3/4}$ is usually taken to give the *optimum (point) resolution* ($0.67C^{1/4}\lambda^{3/4}$). This means that the considered passband extends over the spatial frequency region within which transfer is greater than 70%. Beams with k larger than the first crossover are still linearly imaged, but with reverse contrast. Images formed by beams transferred with opposite phases cannot be intuitively interpreted.

Information limit

Information limit: corresponds to the highest spatial frequency still appreciably transmitted to the intensity spectrum. This resolution is related to the finest detail that can actually be seen in the image (which however is only interpretable using image simulation). For a thin specimen, such limit is determined by the cut-off of the transfer function due to spread of focus and beam convergence (usually taken at $1/e^2$ or at zero).

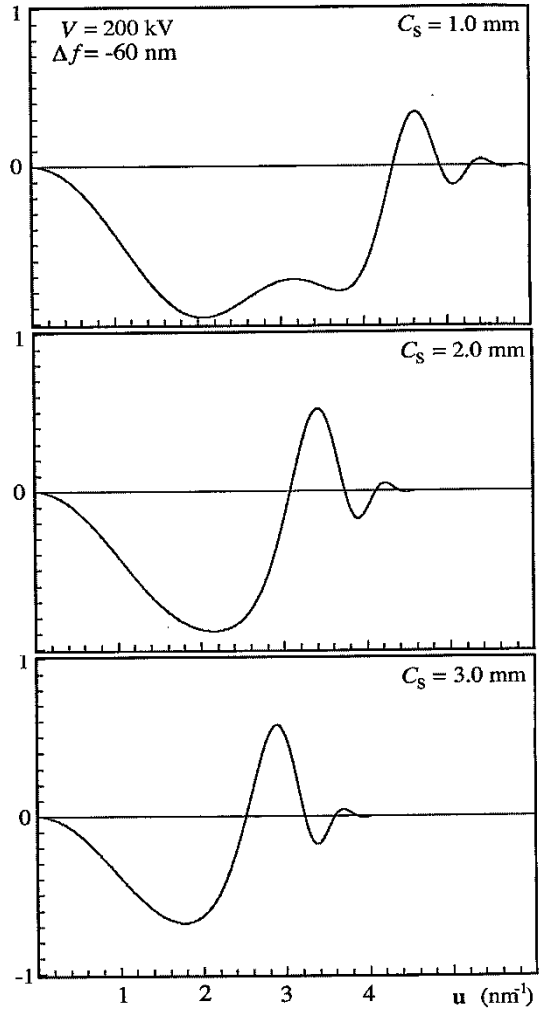
These damping effects are represented by E_Δ or E_{tc} a *temporal coherency envelope* (caused by chromatic aberrations, focal and energy spread, instabilities in the high tension and objective lens current), and E_α or E_{sc} is the spatial coherency_*envelope* (caused by the finite incident beam convergence, i.e., the beam is not fully parallel).

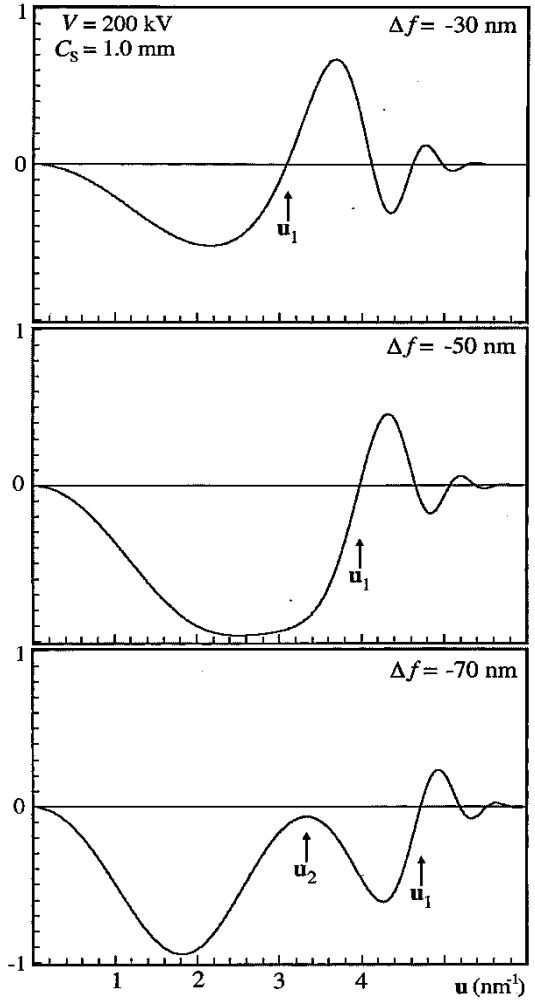
The Information limit goes well beyond point resolution limit for FEG microscopes (due to high spatial and temporal coherency). For the microscopes with thermionic electron sources (LaB6 and W), the info limit usually coincides with the point resolution.

The use of FEG sources minimises the loss of spatial coherence. This helps to increase the information limit resolution in the case of lower voltage (≤ 200 kV) instruments, because in these cases the temporal coherence does not usually play a critical role. However the point resolution is relatively poor due to the oscillatory behavior of the CTF. On the other hand, with higher voltage instruments, due to the increased brightness of the source, the damping effects are always dominated by the spread of focus and FEG sources do not contribute to an increased information limit resolution.

The effect of different C_s and Δf on the damped CTF

$$\sin\chi = \sin(\pi\Delta f\lambda q^2 + \frac{1}{2}\pi C_s\lambda^3 q^4)$$





3.2.1 The contrast transfer function

The fourier transform of the specimen exit-wave modulated by the properties of the imaging system of the TEM at the back focal plane of the objective lens can be represented by a fourier wave function. This is commonly known as microscope specific contrast transfer function, as given by equation 3.4 [70]

Envelope Functions

$$F(q) = \psi(q,0) \cdot exp[i(\frac{1}{2}\pi\lambda^3 q^4 C_s + \pi\lambda\Delta f \cdot q^2)] \cdot [E_s(q) \cdot E_t(q) \cdot E_i(q) \cdot A(q)]^{\frac{1}{2}} \qquad (3.4)$$

Here, $\psi(q,0)$ represents the amplitude of the complex specimen exit-wave function, q the spatial frequency, Δf represents the defocus of the objective lens, C_s the coefficient of spherical aberration. E_s and E_t represent the envelope functions of spatial and temporal coherence, E_i the instrumental instabilities and A represents the effect of objective aperture size.

The Contrast Transfer Function:

Envelope Functions

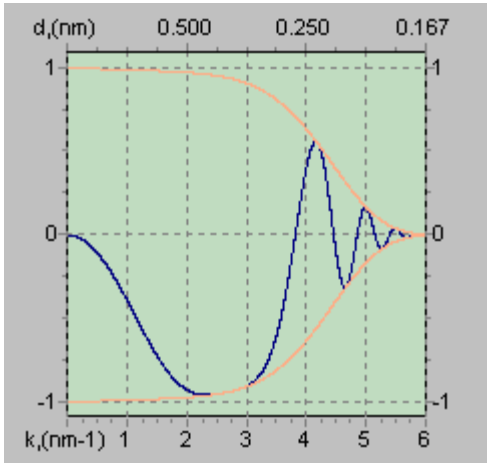
$$F(q) = \psi(q,0) \cdot exp[i(\frac{1}{2}\pi\lambda^3 q^4 C_s + \pi\lambda\Delta f \cdot q^2)] \cdot [E_s(q) \cdot E_t(q) \cdot E_i(q) \cdot A(q)]^{\frac{1}{2}} \qquad (3.4)$$

Phase Contrast Transfer Function:

For Weak Phase Object Approximation:

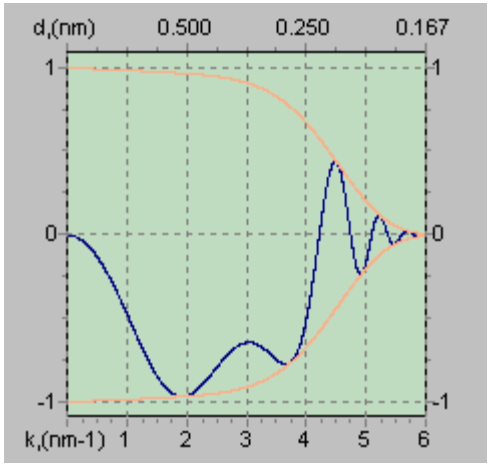
$$B(q) = \sin(\phi(q)) = \sin(\frac{1}{2}\pi\lambda^3 q^4 C_s + \pi\lambda\Delta f \cdot q^2) \cdot [E_s(q) \cdot E_t(q) \cdot E_i(q) \cdot A(q)] \qquad (3.5)$$

Scherzer defocus



$\Delta f = -(C_s\lambda)^{1/2}$

Scherzer condition



$\Delta f = -1.2(C_s\lambda)^{1/2}$

Extended Scherzer condition

http://www.maxsidorov.com/ctfexplorer/webhelp/effect_of_defocus.htm

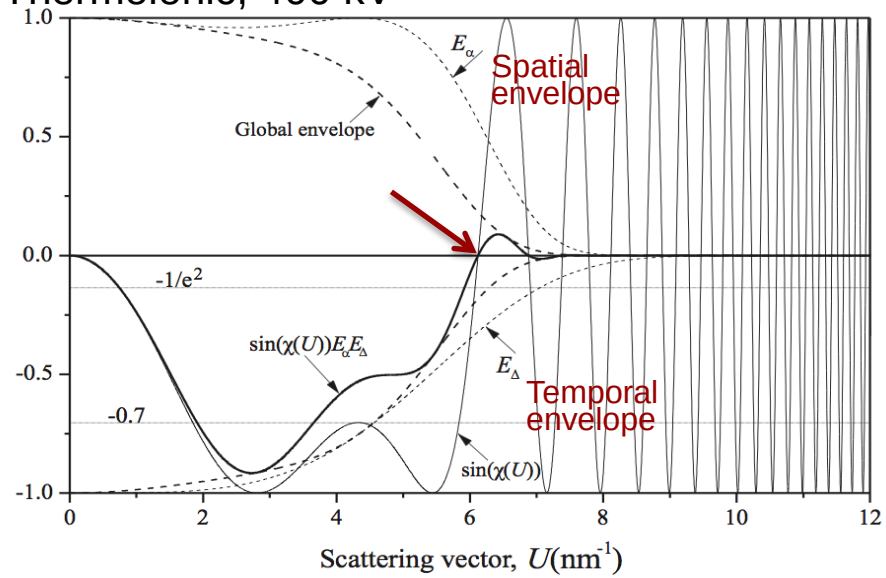
Damped contrast transfer function

Microscope examples

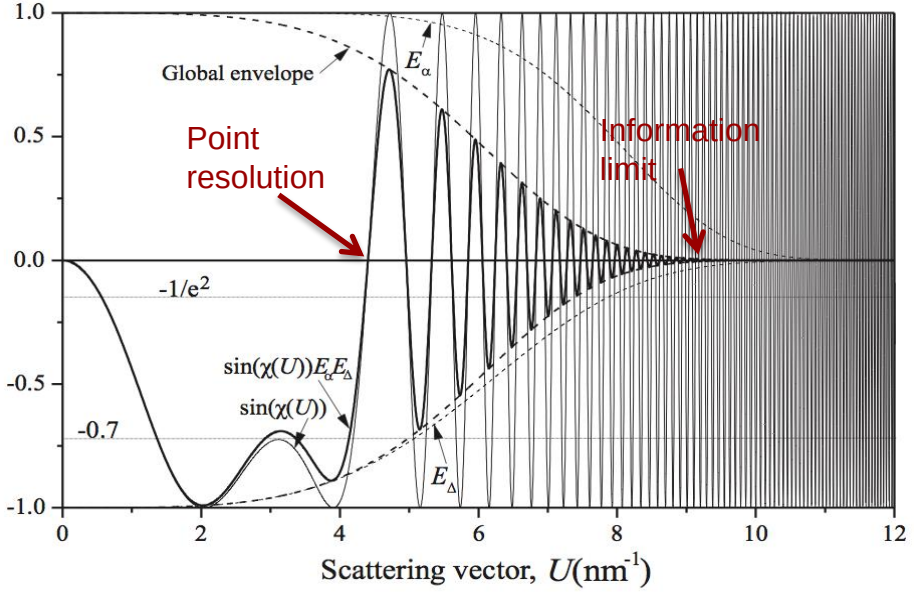
Configuration	JEOL 4000EX/II (Top-entry)	JEOL 2010F (Side-entry)
Emission	LaB_6 filament	Field emission gun
Operating voltage (kV)	400	200
Spherical aberration coefficient (mm)	0.97	~1.00
Spread of focus (nm)	7.8	4.0
Beam convergence angle (mrad)	0.8	0.1
Information limit resolution (nm)	0.14	0.11
Point Resolution (nm)	0.17	0.23
Optimum defocus (nm)	-48.9	-61.0

(Scherzer)

Thermoionic, 400 kV

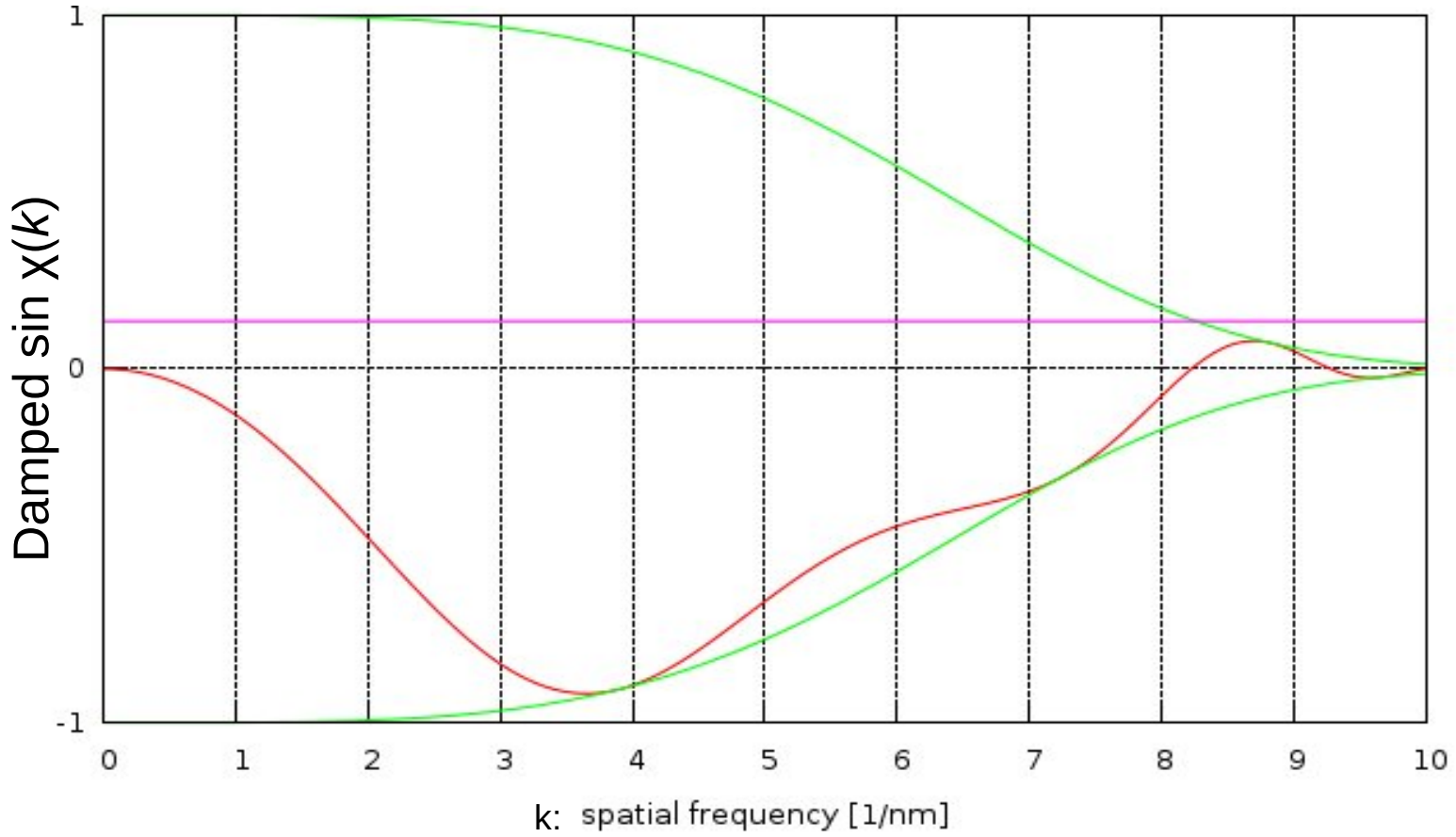


FEG, 200 kV



Spherical aberration correction

In every uncorrected electron microscope the reachable point resolution is much worse than the optimum information limit. **Using an electron microscope with spherical aberration correction allows for optimizing the spherical aberration coefficient and the defocus so that the point resolution equals the information limit.**



parameters: λ=0.0025 nm (200 kV), c_s =0.159 mm, c_c =1.6 mm, Δf=23.92 nm, ΔE=0.7 eV, E=300 kV

HRTEM image simulation

HRTEM image simulation

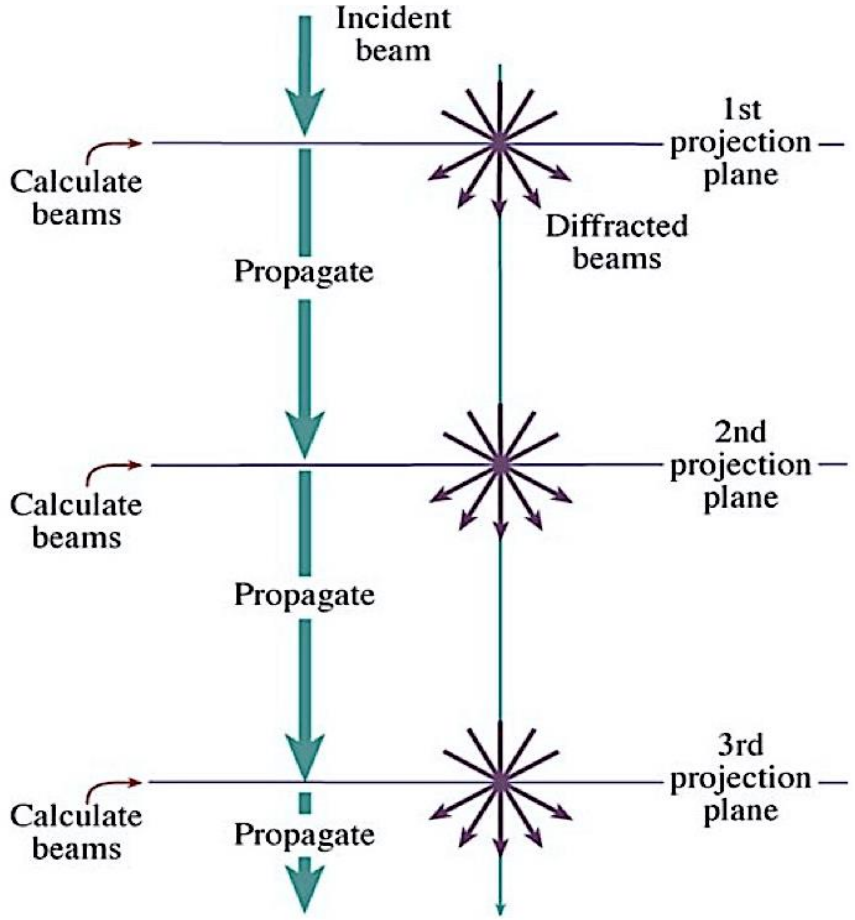
Simulation of HRTEM images is necessary due to the loss of phase information when obtaining an experimental image, which means the object structure can not be directly retrieved. Instead, one assumes a structure (perfect crystal or crystalline material containing defects), simulates the image, matches the simulated image with the experimental image, modifies the structure, and repeats the process. The difficulty is that the image is sensitive to several factors:

- Precise alignment of the beam with respect to both the specimen and the optic axis
- Thickness of the specimen
- Defocus of the objective lens
- Chromatic aberration which becomes more important as the thickness increases
- Coherence of the beam
- Other factors such as the intrinsic vibration in the material which we try to take account of through the Debye-Waller factor

Multislice method

The basic multislice approach used in most of the simulation packages is to section the specimen into many slices, which are normal to the incident beam.

The potential within a slice is projected onto the first projection plane; this is the phase grating. We calculate the amplitudes and phases for all the beams generated by interacting with this plane and then propagate all the diffracted beams through free space to the next projection plane, and repeat the process.



Williams and Carter

• END •