Image formation in Conventional TEM

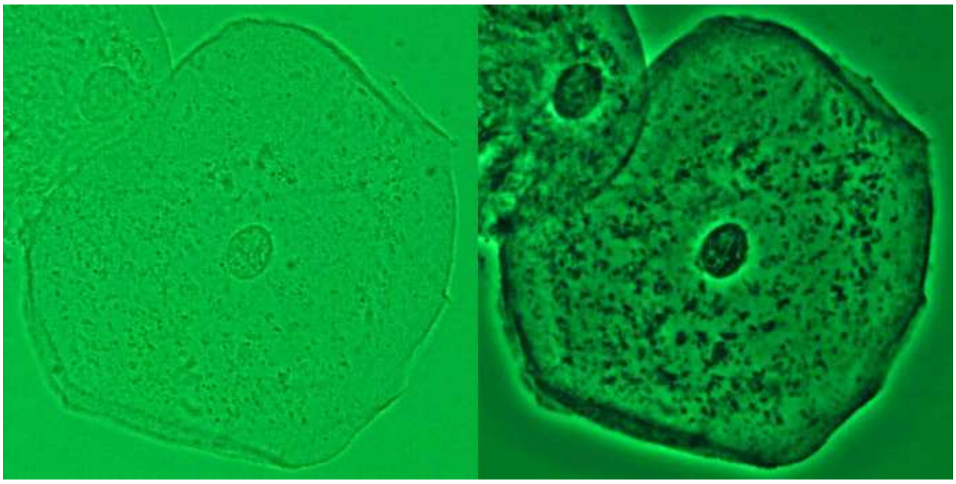
MSN510 Class notes

Mostly compiled from other sources

- UNAM BILKENT -

Phase Contrast

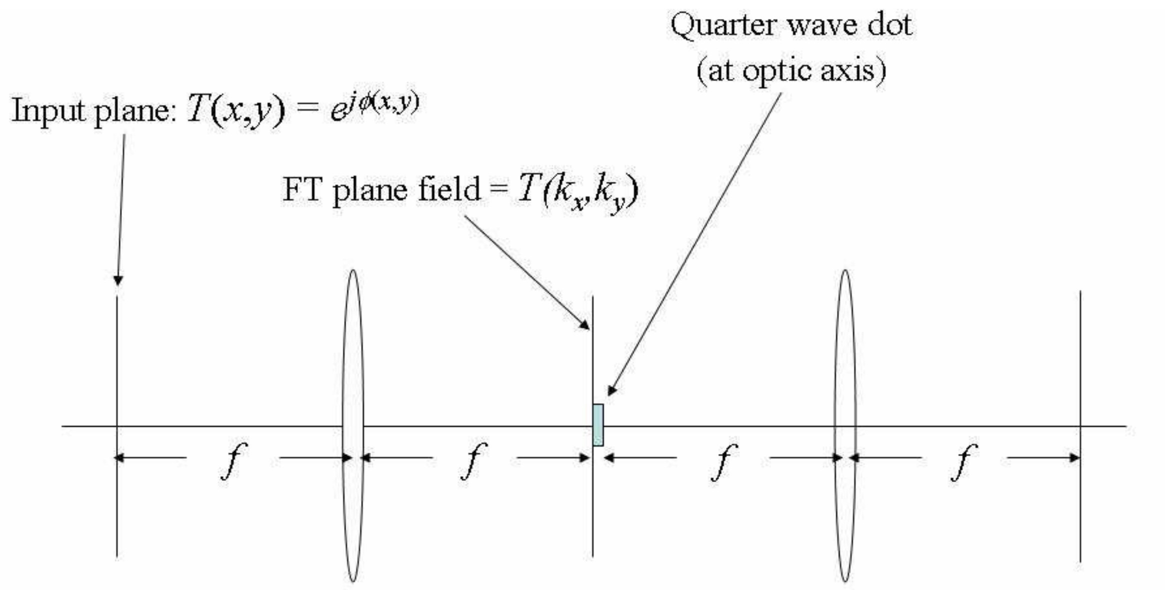
- Converts phase change to Amplitude change



http://micro.magnet.fsu.edu/primer/techniques/phasecontrast/phaseindex.html

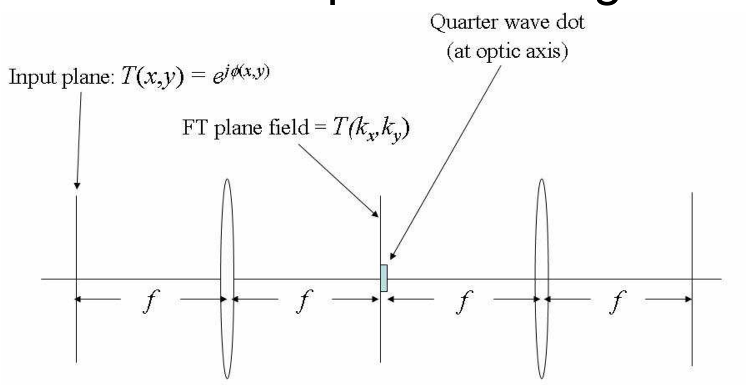
Phase Contrast

- Converts phase change to Amplitude change



Implementing Phase Contrast Using 4F Correlator

- Converts phase change to Amplitude change



Implementing Phase Contrast Using 4F Correlator

$$T(x,y) = e^{j\phi(x,y)}$$

$\varphi(x,y) << 1$

$$T(x,y) = e^{j\phi(x,y)} \cong 1 + j\phi(x,y)$$

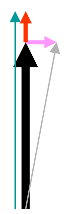
Without PC optics

PSF(*kx*,*ky*) is the Point spread function (PSF)

$$T(k_x,k_y) = PSF(k_x,k_y) + j\Phi(k_x,k_y)$$

$$E(k_x,k_y) = jPSF(k_x,k_y) + j\Phi(k_x,k_y)$$

$$E(x,y) = 1 + \phi(x,y)$$



With PC optics

Proper Choice of the phase shift reverses contrast

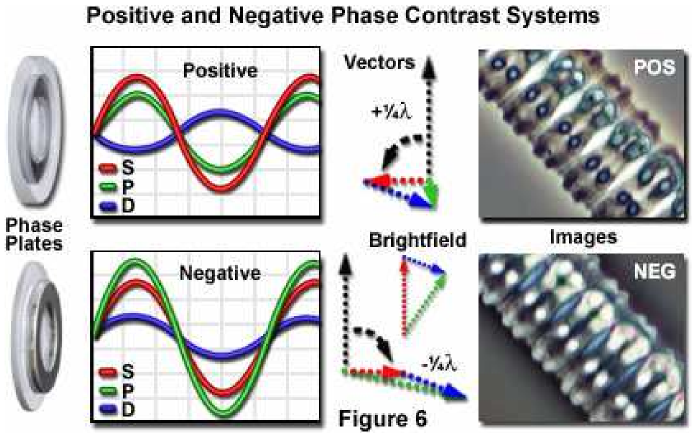


Figure 6

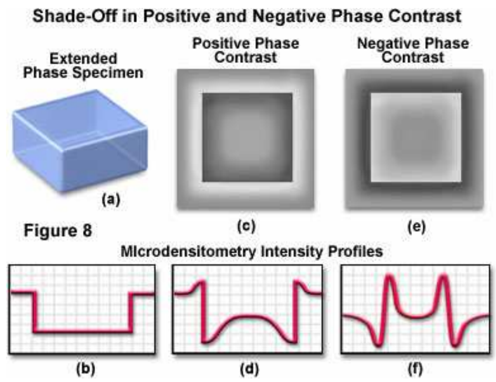


Figure 8

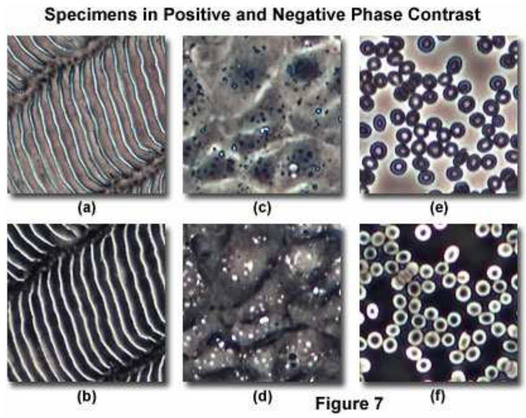
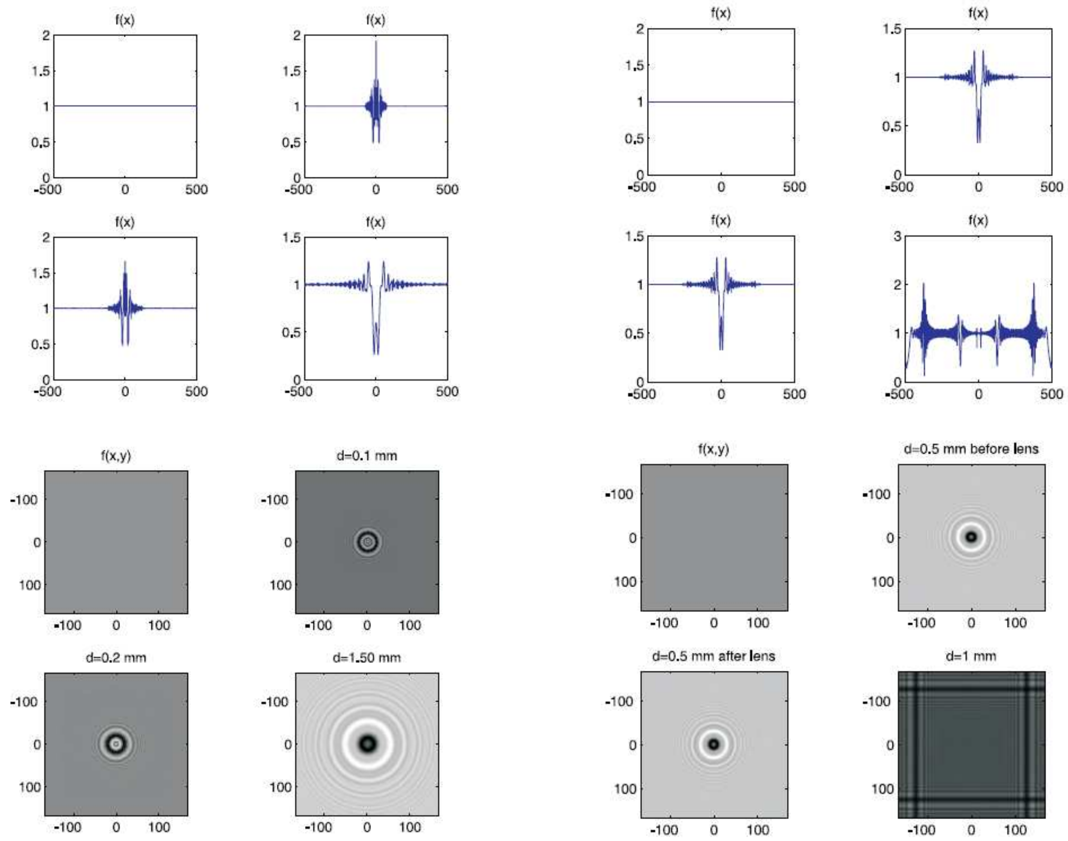
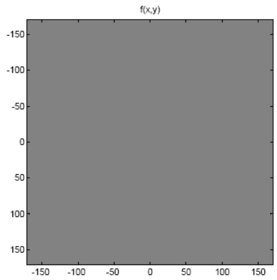


Figure 7

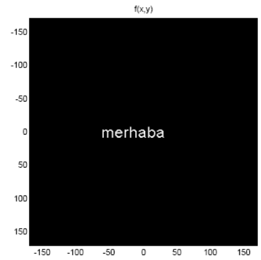
Phase Contrast



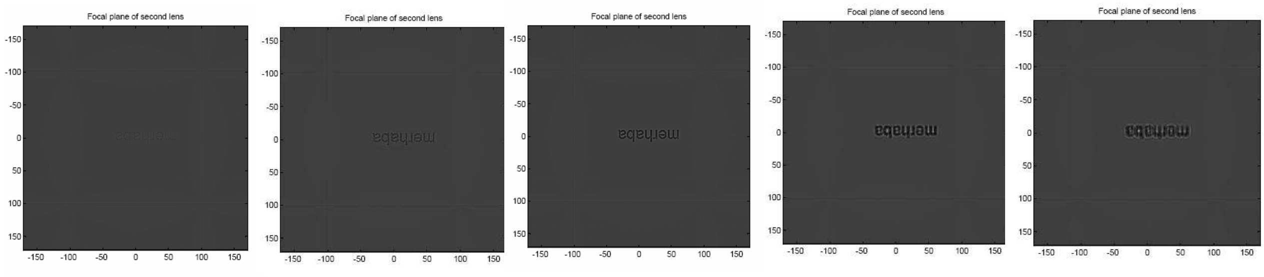
Phase Contrast convert to amplitude contrast with defocusing



Amplitude of object



Phase of object



0 defocus

Increasing defocus

Contrast Transfer Function

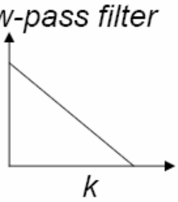
The contrast transfer function (CTF) is the Fourier Transform of the point spread function (PSF)

The CTF describes the response of the system to an input plane wave.
By convention the CTF is normalized to the response at zero frequency (i.e. DC level)

$$\widetilde{H}(k) = \frac{H(k)}{H(0)}$$

A low-pass filter

$\widetilde{H}(k)$

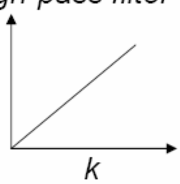


(division by k in Fourier Space ->integration in real space)

smoothing

A high-pass filter

$\widetilde{H}(k)$



(multiplication by k in Fourier Space ->differentiation in real space)

Edge-enhancing

Coherent vs. Incoherent Imaging

(Kirkland, Chapter 3.3)

Lateral Coherence of the Electron Beam for an angular spread β_{max} (Born&Wolf): $$\Delta x_{coh} \approx \frac{0.16\lambda}{\beta_{\max}}$$

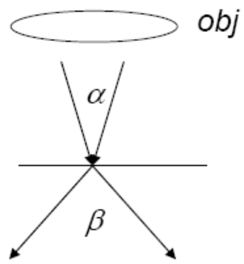


Image resolution $$d \approx \frac{\lambda}{\alpha_{\max}}$$

Combining these 2 formula we get:

Coherent imaging: $\beta_{\max} << 0.16\alpha_{\max}$

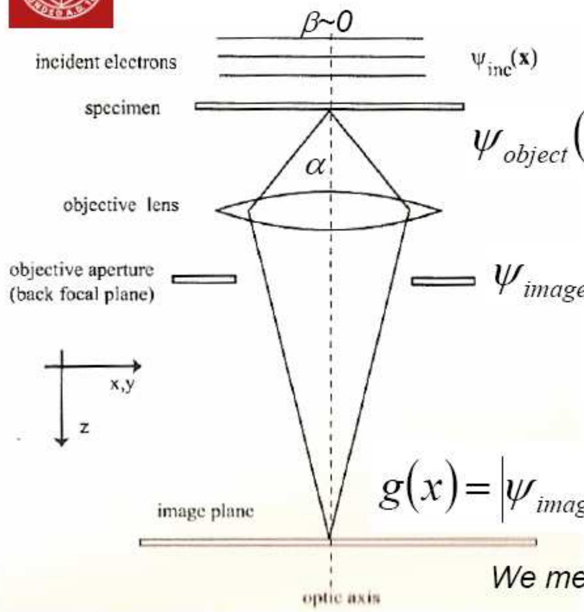
Wave Interference inside Δx_{coh} *allows us to measure phase changes as wavefunctions add:* $|\psi_a + \psi_b|^2 = |\psi_a|^2 + |\psi_b|^2 + \psi_a\psi_b^* + \psi_b\psi_a^*$

Incoherent imaging: $\beta_{\max} >> 0.16\alpha_{\max}$ *(usually* $\beta_{\max} > 3\alpha_{\max}$ *)*

No interference, phase shifts are not detected. Intensities add $|\psi_a|^2 + |\psi_b|^2$

Coherent Imaging

(Kirkland 3.1)



$\psi_{object}(x)$

$\psi_{image}(k)$

Lens has a PSF A(x)

$$\psi_{image}(x) = \psi_{object}(x) \otimes A(x)$$

$$\downarrow$$

$$\psi_{image}(k) = \psi_{object}(k) \cdot A(k)$$

$$g(x) = |\psi_{image}(x)|^2$$

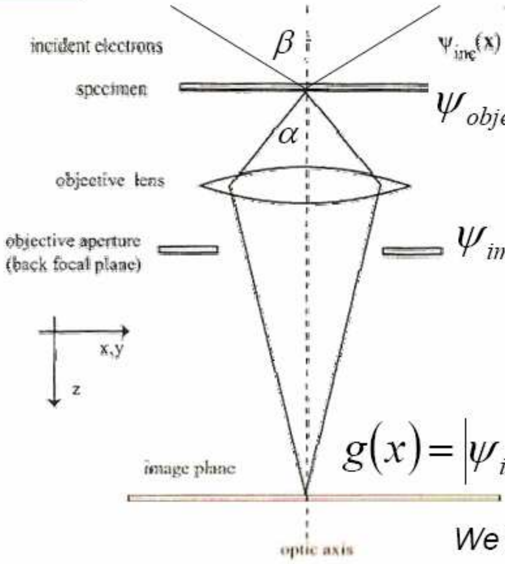
We measure the intensity, not the wavefunction

$$g(x) = |\psi_{object}(x) \otimes A(x)|^2$$

Convolve wavefunctions, measure intensities

Incoherent Imaging (Kirkland 3.4)

Lost phase information, only work with intensities



$$\psi_{object}(x)$$

$$\psi_{image}(k)$$

$$g(x) = \left|\psi_{image}(x)\right|^2$$

Lens has a PSF $\left|A(x)\right|^2$

$$\left|\psi_{image}(x)\right|^2 = \left|\psi_{object}(x)\right|^2 \otimes \left|A(x)\right|^2$$

$$\downarrow$$

$$\psi_{image}(k) = \left[\psi_{object}(k) \otimes \psi^*_{object}(k)\right] \cdot \underbrace{\left[A(k) \otimes A^*(k)\right]}_{CTF}$$

We measure the intensity, not the wavefunction

$$g(x) = \left|\psi_{object}(x)\right|^2 \otimes \left|A(x)\right|^2$$

Convolve intensities, measure intensities

Coherent vs Incoherent Imaging

	Coherent	*Incoherent*
Point Spread Function	$A(x)$	$\left\|A(x)\right\|^2$
Contrast Transfer Function	*Phase Object* $\mathrm{Im}\left[A(k)\right]$ *Amplitude Object* $\mathrm{Re}\left[A(k)\right]$	$\left\|A(k) \otimes A^*(k)\right\|^2$
We measure	$g(x) = \left\|\psi_{object}(x) \otimes A(x)\right\|^2$	$g(x) = \left\|\psi_{object}(x)\right\|^2 \otimes \left\|A(x)\right\|^2$

An Arbitrary Distortion to the Wavefront can be expanded in a power series

(Either Zernike Polynomials or Seidel aberration coefficients)

Zernike Polynomials

$$\chi(\rho,\theta') = = Z_0 - Z_3 + Z_8 \quad \text{piston}$$
$$+\rho\sqrt{(Z_1-2Z_6)^2+(Z_2-2Z_7)^2}$$
$$\times\cos\left[\theta' - \tan^{-1}\left(\frac{Z_2-2Z_7}{Z_1-2Z_6}\right)\right] \quad \text{tilt}$$
$$+\rho^2(2Z_3-6Z_8 \pm \sqrt{Z_4^2+Z_5^2}) \quad \text{focus}$$
$$\pm 2\rho^2\sqrt{Z_4^2+Z_5^2}\cos^2\left[\theta' - \frac{1}{2}\tan^{-1}\left(\frac{Z_5}{Z_4}\right)\right] \quad \text{astigmatism}$$
$$+3\rho^3\sqrt{Z_6^2+Z_7^2}\cos\left[\theta' - \tan^{-1}\left(\frac{Z_7}{Z_6}\right)\right] \quad \text{coma}$$
$$+6\rho^4 Z_8. \quad \text{spherical}$$

TABLE IV
ABERRATIONS CORRESPONDING TO THE FIRST NINE ZERNIKE TERMS

Z_0	piston
Z_1	x-tilt
Z_2	y-tilt
Z_3	focus
Z_4	astigmatism @ 0° & focus
Z_5	astigmatism @ 45° & focus
Z_6	coma & x-tilt
Z_7	coma & y-tilt
Z_8	spherical & focus

J.C. Wyant, K. Creath, APPLIED OPTICS AND OPTICAL ENGINEERING, VOL. XI

Phase Shift in a Lens

(Kirkland, Chapter 2.4)

Electron wavefunction in focal plane of the lens

$$\varphi(\alpha) = e^{i\chi(\alpha)}$$

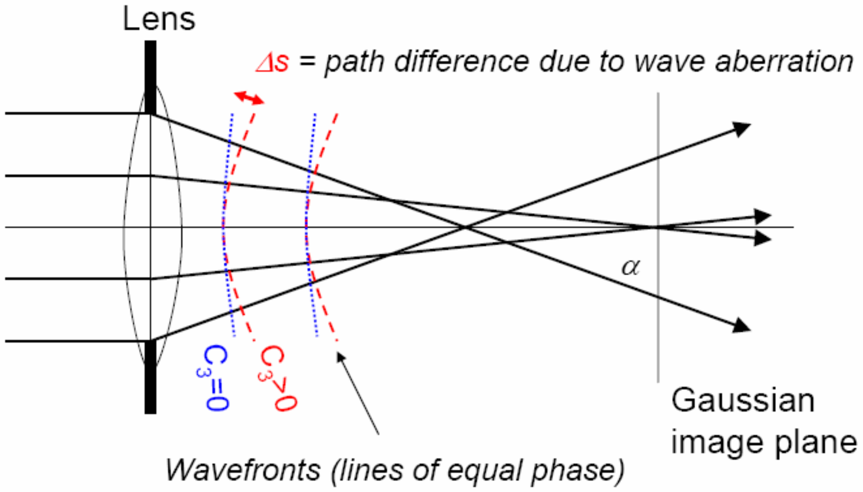
Where the phase shift from the lens is

$$\chi(\alpha) = \frac{2\pi}{\lambda}\left(\frac{1}{4}C_3\alpha^4 - \frac{1}{2}\Delta f\alpha^2\right)$$

Keeping only spherical aberration and defocus

$$A(\vec{k}) = \begin{cases} e^{i\chi(k)}, & |\vec{k}| < k_{\max} \\ 0, & |\vec{k}| > k_{\max} \end{cases}$$

Spherical Aberration (C_3) as a Phase Shift



Phase shift from lens aberrations: $\chi(\alpha) = \frac{2\pi}{\lambda}\Delta s(\alpha)$

(remember wave exp[i(2π/λ) x] has a 2π phase change every λ)

For spherical aberration $\Delta s(\alpha) = \frac{1}{4}C_3\alpha^4$ *but there are other terms as well*

David Muller 2006

Michael A. O'Keefe* and Yang Shao-Horn**

In the HRTEM, the image is recorded with an intensity, I (x), which is the square of the complex image amplitude, or electron wave, ψ(x) at the image plane:

$$I(x) = \psi(x)\ \psi^*(x) \qquad (1)$$

Fourier transformation of this equation gives the image intensity spectrum as the auto-correlation function of the image amplitude spectrum, Ψ(u)

$$I(u) = \Psi^*(-u) \otimes \Psi(u) \qquad (2)$$

where ⊗ represents convolution.

The convolution may be written out as a sum over all pairs of amplitude spectrum components, Ψ(u) that contribute to the image, in the form

$$I\ (u) = \sum_{u'} \Psi\ (u')\ .\ \Psi^*(u'-u) \qquad (3)$$

where each product term represents the contribution to the image intensity spectrum of the interference of any complex diffracted beam amplitude Ψ (u') with (the conjugate of) all the complex diffracted beam amplitudes Ψ*(u'-u).

Phase Shift in a Lens

(Kirkland, Chapter 2.4)

Electron wavefunction in focal plane of the lens

$$\varphi(\alpha) = e^{i\chi(\alpha)}$$

Where the phase shift from the lens is

$$\chi(\alpha) = \frac{2\pi}{\lambda}\left(\frac{1}{4}C_3\alpha^4 - \frac{1}{2}\Delta f\alpha^2\right)$$

Keeping only spherical aberration and defocus

$$A(\vec{k}) = \begin{cases} e^{i\chi(k)}, & \left|\vec{k}\right| < k_{\max} \\ 0, & \left|\vec{k}\right| > k_{\max} \end{cases}$$

Phase changes from the objective lens are imposed on the specimen exit-surface wave Ψ_e (u), to produce the image amplitude spectrum wave Ψ (u). The phase changes are described via an objective lens phase function χ(u), such that

$$\Psi(u) = \Psi_E(u).\exp\{-i\chi(u)\} \quad (4)$$

Then the image intensity spectrum is given by

$$I(u) = \sum_{u'} \Psi_E(u').\exp\{-i\chi(u')\}.\Psi_E^*(u'-u).\exp\{+i\chi(u'-u)\}$$

$$\chi(u) = \pi\varepsilon\lambda|u|^2 + \pi C_S\lambda^3|u|^4/2 \quad (5)$$

Abbé Concept of Image Formation

High spatial frequencies in the object do not pass through the lens aperture; low frequencies do. The frequencies that pass through the lens for a Fourier transform (with a phase factor) at the focal pland (source image plane) before passing on to the image plane.

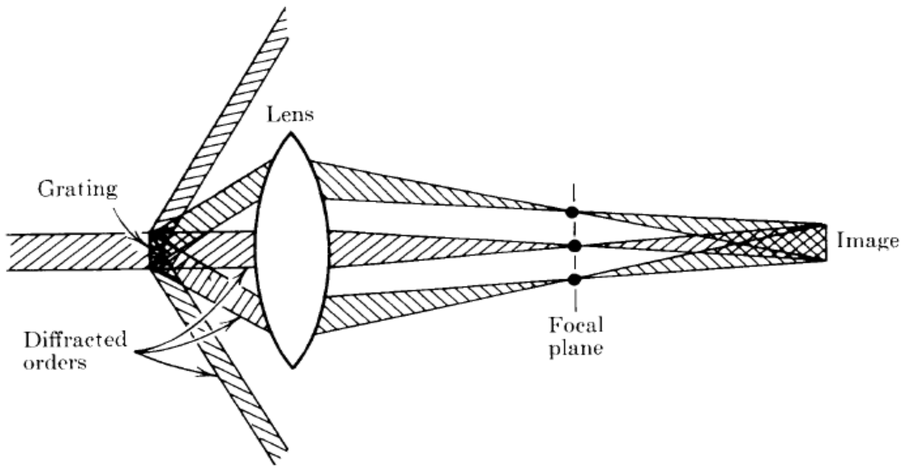


Figure 6-2 The Abbe theory of image formation.

With non-linear terms excluded from eqn.5, the uth component of the "linear-image" intensity spectrum contains only u and -u diffracted-beam interference with the zero beam

$$I_L(u) = \Psi_E\,(u)\,\exp\{-i\chi(u)\}\,.\,\Psi_E^*(0) + \Psi_E\,(0).\Psi_E^*(-u)\,\exp\{+i\chi(-u)\} \tag{6}$$

$\Psi(0)$ has a weight that is close to unity for a weakly-scattering specimen. Since it is present for all the interference terms and can be normalized out, we can write

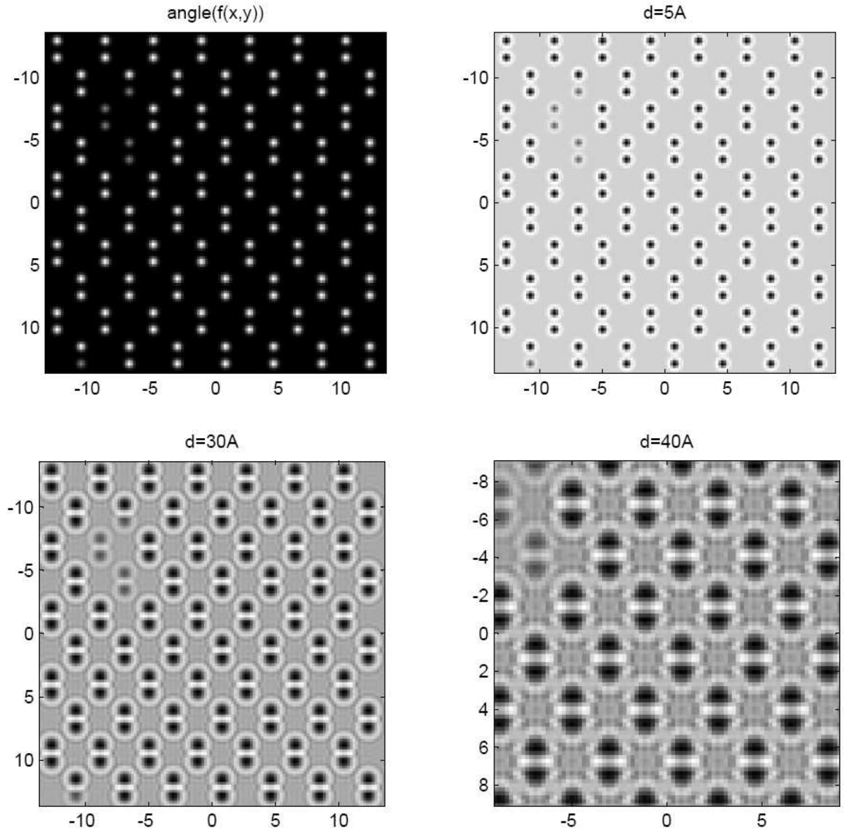
$$I_L(u) = \Psi_E\,(u).\exp[-i\chi(u)] + \Psi_E^*(-u).\exp[+i\chi(-u)] \tag{7}$$

The electron wave at the specimen exit surface is a function of the (projected) specimen structure. The

function of the (projected) specimen structure. The major effect of elastic scattering of the electrons within the specimen occurs on the phase of the electron wave traversing the specimen – the specimen behaves as a “phase object”. Thus, information about the (projected) spatial distribution of specimen potential $\phi_p(x)$ and specimen thickness H is encoded in the phase of the electron wave, which can be written

$$\psi_E(x) = \exp\{-\,i\,\sigma\,\phi_p(x)\,H\} \tag{8}$$

Electron wavefunction after exit

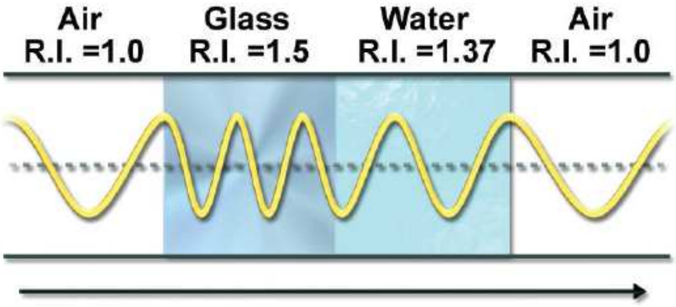


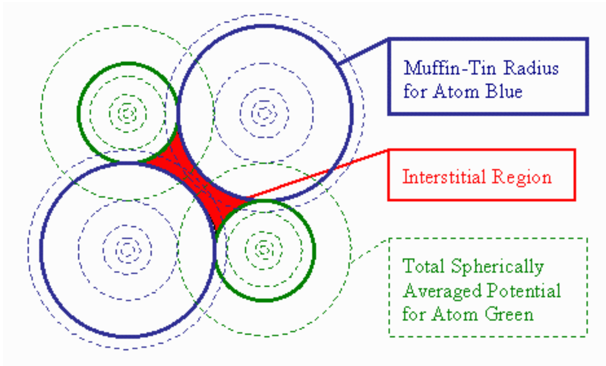
For our weakly-scattering specimen, the majority of the elastically-scattered electrons will undergo kinematic (single) scattering. Neglecting dynamical diffraction, the direct-space electron wave at the specimen exit-surface of this "weak phase object" can then be written

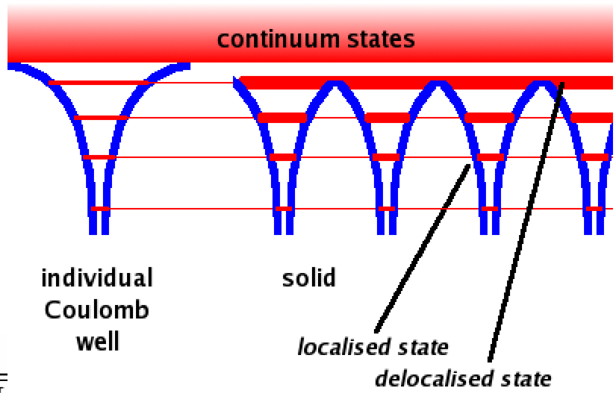
$$\psi_E(x) = 1 - i\,\sigma\,\phi_p(x)\,H \qquad (9)$$

where σ is the interaction coefficient, $\phi_p(x)$ is the specimen potential projected in the incident electron beam direction, and H is the specimen thickness. In Fourier space

LIGHT







Electrons

$$\lambda = \frac{h}{\sqrt{2m_0 eU}} \frac{1}{\sqrt{1 + \frac{eU}{2m_0 c^2}}}$$

direction, and H is the specimen thickness. In Fourier space

$$\Psi_E(u) = \delta(u) - i\ \sigma\ V(u)\ H \qquad (10)$$

where V(u) is the (complex) Fourier component, with spatial frequency u, of the (real) projected potential $\phi_p(x)$.

When the (reciprocal-space) exit-surface wave (10) is included, the expression for the linear image intensity spectrum (7) becomes

$$I_L(u) = \delta(u) - i\ \sigma\ V(u)\ H \exp[i\chi(u)] + i\ \sigma\ V^*(-u)\ H \exp[-i\chi(-u)] \qquad (11)$$

$$I_L(u) = \delta(u) - i\,\sigma\,V(u)\,H\,\exp[i\chi(u)] + i\,\sigma\,V^*(-u)\,H\,\exp[-i\chi(-u)] \tag{11}$$

Then, since $\{\exp[i\chi(u)] - \exp[-i\chi(-u)]\}$ is equal to $2i\sin\chi(u)$ for a round lens, and $V^*(-u)$ is equal to $V(u)$ for a real potential, the image intensity spectrum for such a "linear" (or "weak-phase object") image is reduced to

$$I_L(u) = \delta(u) + 2\,\sigma\,V(u)\,H\,\sin\chi(u) \tag{12}$$

Thus the magnitude of the uth term in the image intensity spectrum is just proportional to $V(u)$, which is the uth Fourier coefficient of the projected potential, and to $\sin\chi(u)$, the value of the phase-contrast transfer function (CTF) at the corresponding value of $|u|$.

By choosing a value of defocus at which $\sin\chi(u)$ is approximately equal to –1 (Scherzer or optimum defocus), it is possible to have each term in the intensity spectrum proportional to (the negative of) the corresponding Fourier coefficient of the projected potential. An inverse Fourier transformation back into direct space yields image intensity proportional to the negative magnitude of the projected potential. Peaks in the potential at the atom positions will produce dips in the image intensity; the image will show “black atoms”.

$$I_L(x) = 1 - 2\,\sigma\,\phi_p(x)\,H \tag{13}$$

Phase Shift in a Lens

(Kirkland, Chapter 2.4)

Electron wavefunction in focal plane of the lens

$$\varphi(\alpha) = e^{i\chi(\alpha)}$$

Where the phase shift from the lens is

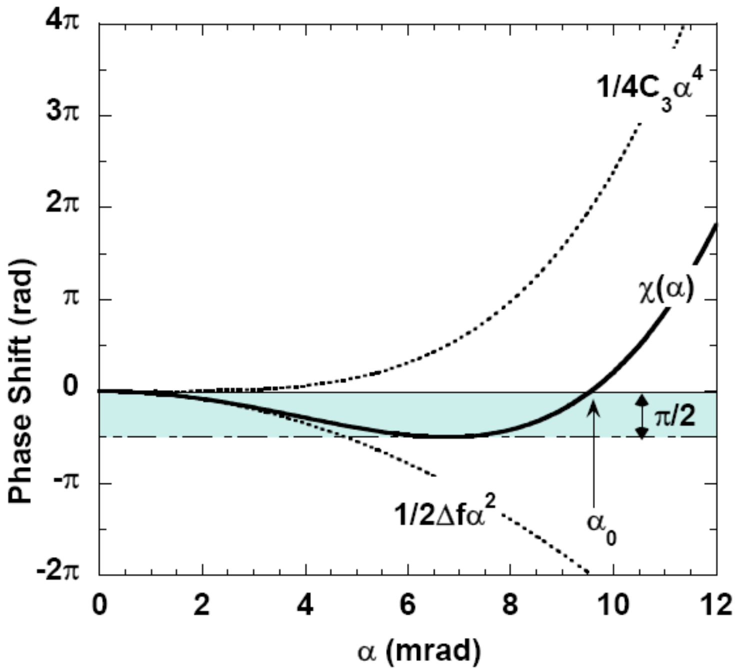
$$\chi(\alpha) = \frac{2\pi}{\lambda}\left(\frac{1}{4}C_3\alpha^4 - \frac{1}{2}\Delta f\alpha^2\right)$$

Keeping only spherical aberration and defocus

$$A(\vec{k}) = \begin{cases} e^{i\chi(k)}, & \left|\vec{k}\right| < k_{\max} \\ 0, & \left|\vec{k}\right| > k_{\max} \end{cases}$$

Optimizing defocus and aperture size for ADF

Goal is to get the smallest phase shift over the largest range of angles



Step 1: Pick largest tolerable phase shift: in EM $\lambda/4=\pi/2$, in light optics $\lambda/10$
Step 2: Use defocus to oppose the spherical aberration shift within the widest $\pi/2$ band
Step 3: Place aperture at upper end of the $\pi/2$ band

Optimizing defocus and aperture size for ADF

Goal is to get the smallest phase shift over the largest range of angles

Step 1: We assume a phase shift <λ/4=π/2 is small enough to be ignored

Step 2: Use defocus to oppose the spherical aberration shift within the widest π/2 band

Optimal defocus: $\Delta f_{opt} = (C_S \lambda)^{1/2}$

Optimal aperture: $\alpha_{opt} = \left(\frac{4\lambda}{C_3}\right)^{1/4}$

Step 3: Place aperture at upper end of the π/2 band & treat as diffraction limited

Minimum Spot size: $d_{\min} \approx \frac{0.61\lambda}{\alpha_{opt}}$

$$d_{\min} = 0.43\, C_3^{1/4} \lambda^{3/4}$$

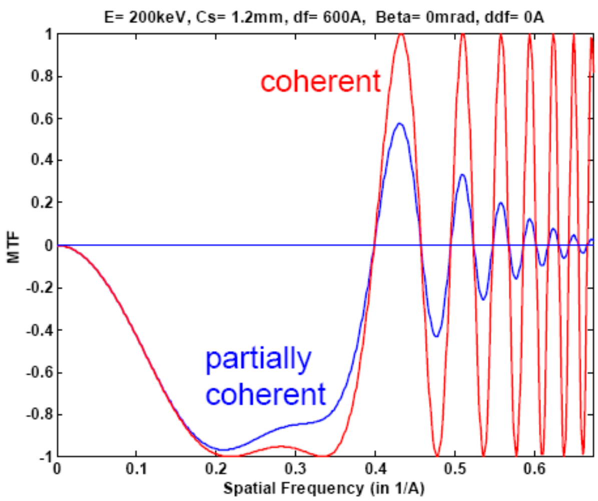
(The full derivation of this is given in appendix A of Weyland&Muller

Contrast Transfer Functions of a lens with Aberrations

Generated with `ctemtf`

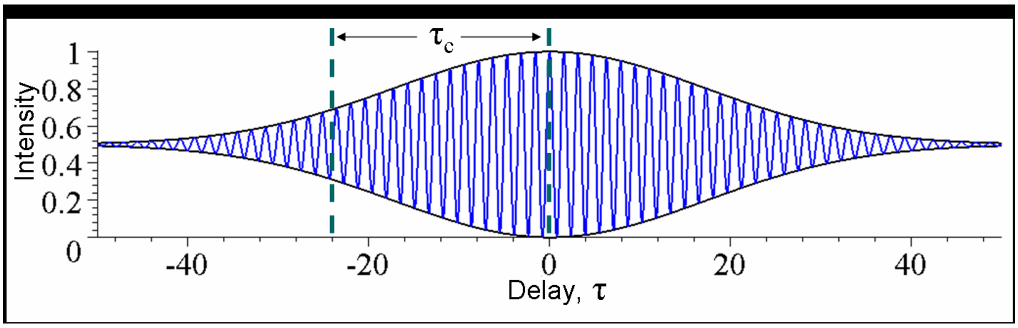
Aperture function of a real lens $A(\vec{k}) = \begin{cases} e^{i\chi(k)}, & |\vec{k}| < k_{\max} \\ 0, & |\vec{k}| > k_{\max} \end{cases}$

Coherent Imaging CTF: $\mathrm{Im}[A(k)] = Sin[\chi(k)]$



Remember Coherence

- A measure of how sinusoidal the wave is
  - Or the length over which it interferes with itself

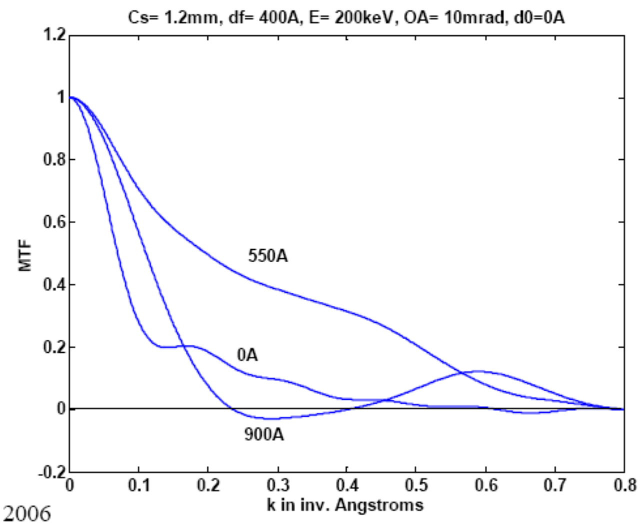


Contrast Transfer Functions of a lens with Aberrations

Generated with **stemtf**

Aperture function of a real lens
$$A(\vec{k}) = \begin{cases} e^{i\chi(k)}, & |\vec{k}| < k_{\max} \\ 0, & |\vec{k}| > k_{\max} \end{cases}$$

Incoherent Imaging CTF: $\left| A(k) \otimes A^*(k) \right|^2$

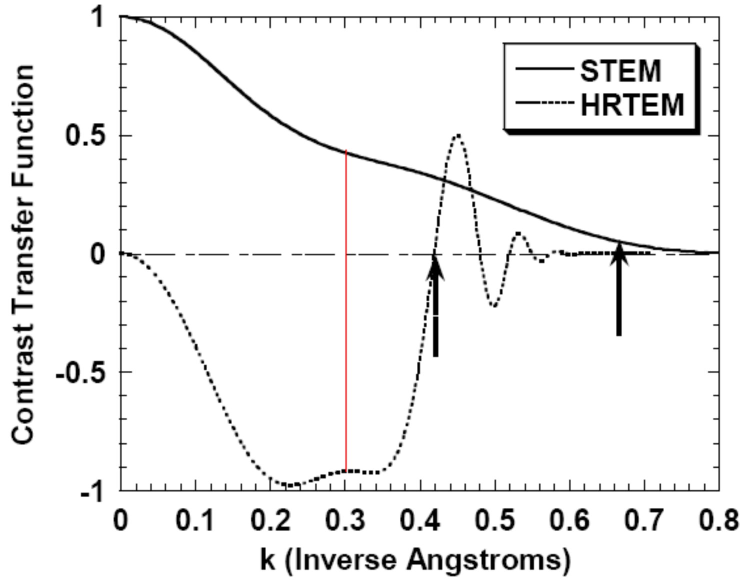


CTF for different defocii

Theorem:
Aberrations will never Increase the MTF For incoherent imaging

Phase vs. ADF Contrast

(JEOL 2010F, C_s=1mm)



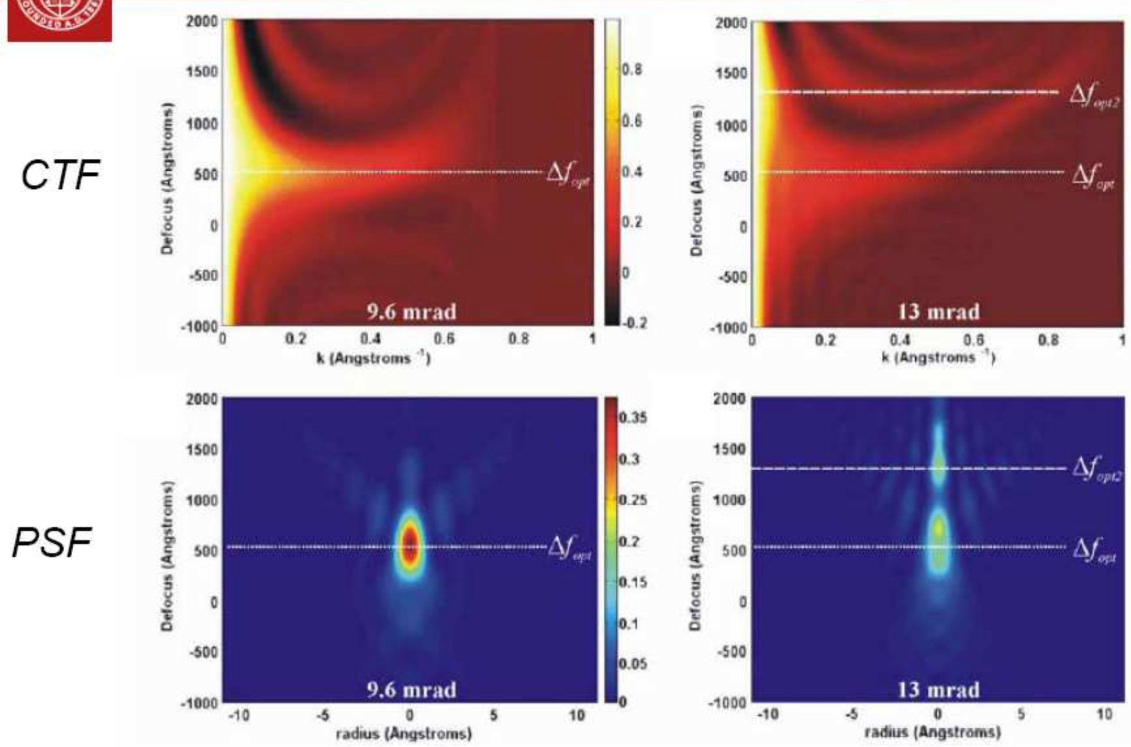
TEM: Bandpass filter:low frequencies removed = artificial sharpening

ADF : Lowpass filter: 3 x less contrast at 0.3 nm than HRTEM

David Muller 2006

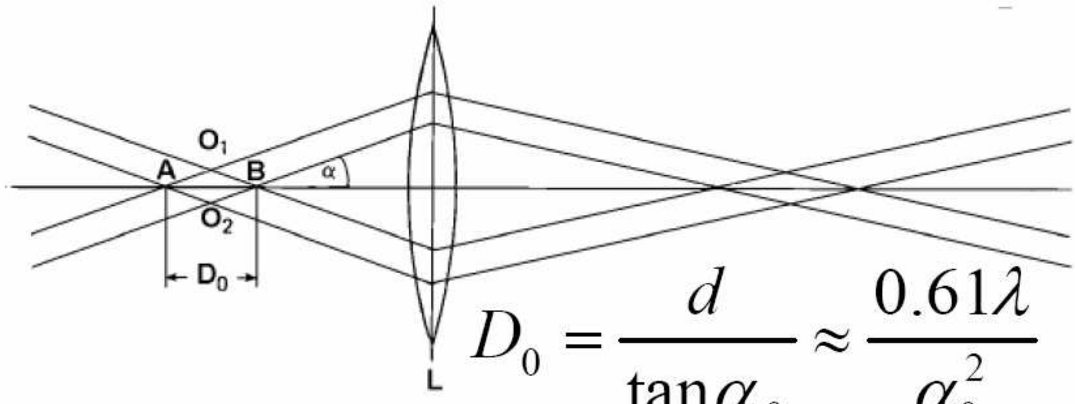
Effect of defocus and aperture size on an ADF-STEM image

(200 kV, C_3=1.2 mm)



David Muller 2006

Depth of Field, Depth of Focus



$$D_0 = \frac{d}{\tan\alpha_0} \approx \frac{0.61\lambda}{\alpha_0^2}$$

Figure 11. Depth of field. Object points O1 **and** O2 **objects are separated by the resolution limit** d **of the lens. Rays from these points cross the axis at** A **and** B **equally. Hence, points between** A **and** B **will look equally sharp, and** AB **is the depth of field** Do **of the lens for a semi-angular aperture α.**

For d=0.2 nm, α=10 mrad, D_0= 20 nm   For d= 2 nm, α=1 mrad, D_0= 2000 nm!

For d= 0.05 nm, α= 50 mrad, D_0= 1 nm!