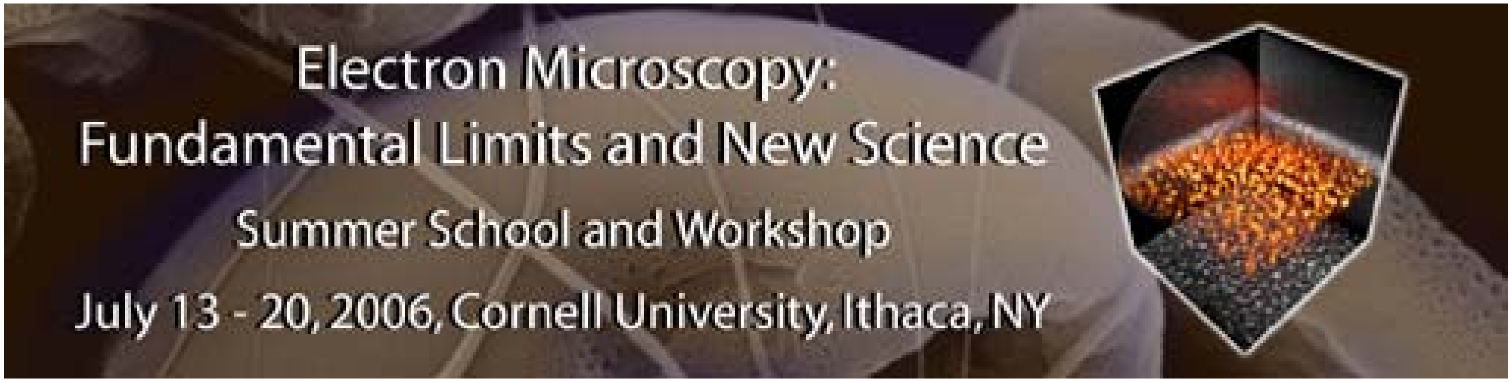
Linear Imaging Approximations

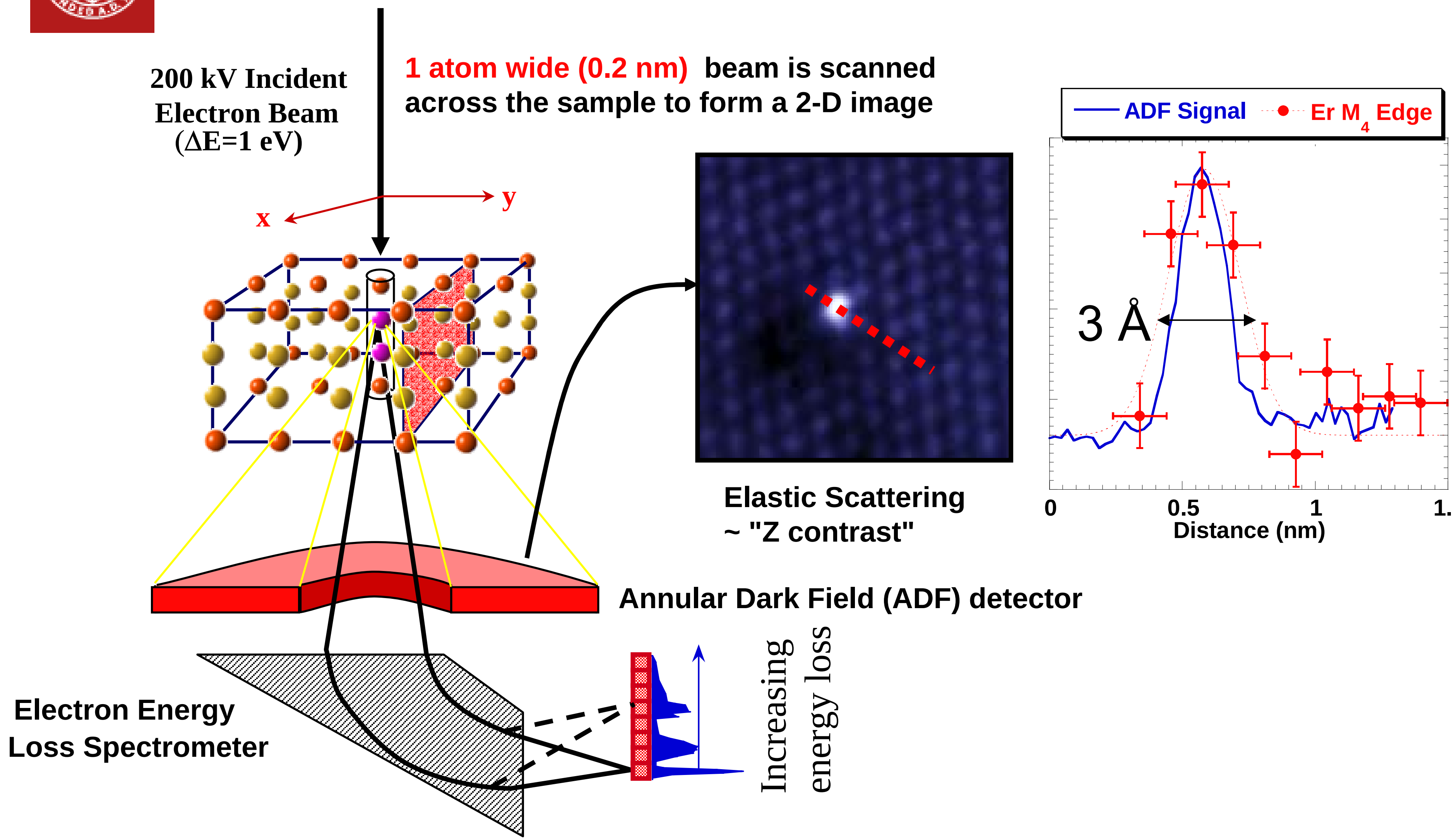


Notes to accompany the lectures delivered by David A. Muller at the Summer School on Electron Microscopy: Fundamental Limits and New Science held at Cornell University, July 13-15, 2006.

Reading and References:

Chapter 1-3 of "*Advanced Computing in Electron Microscopy*" by E. J. Kirkland

Scanning Transmission Electron Microscopy



Single atom Sensitivity: P. Voyles, D. Muller, J. Grazul, P. Citrin, H. Gossmann, *Nature* **416** 826 (2002)
U. Kaiser, D. Muller, J. Grazul, M. Kawasaki, *Nature Materials*, **1** 102 (2002)

Reciprocity *(or STEM vs. CTEM)*

CTEM

Gun

↓

Illumination angle

↓

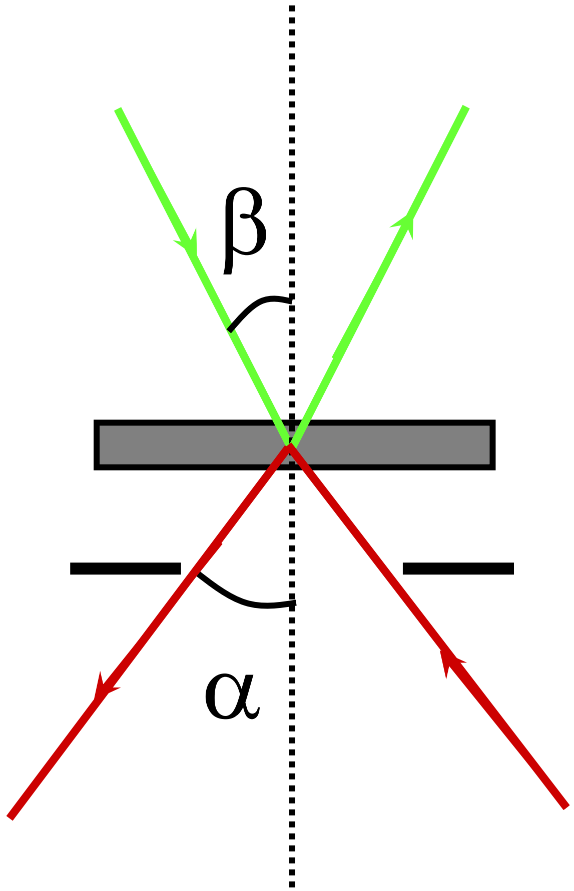
Specimen

↓

Objective Aperture

↓

Viewing Screen



STEM

Detectors

↑

Collector angle

↑

Specimen

↑

Objective Aperture

↑

Gun

Reciprocity (for zero-loss images):

A hollow-cone image in CTEM ⟺ *an annular-dark field image in STEM.*

However: In STEM, energy losses in the sample do not contribute to chromatic aberrations (Strong advantage for STEM in thick specimens)

Reciprocity

<u>Reciprocity:</u> *Electron intensities and ray paths in the microscope remain the same if (i) the direction of rays is reversed, and (ii) the source and detector are interchanged.*

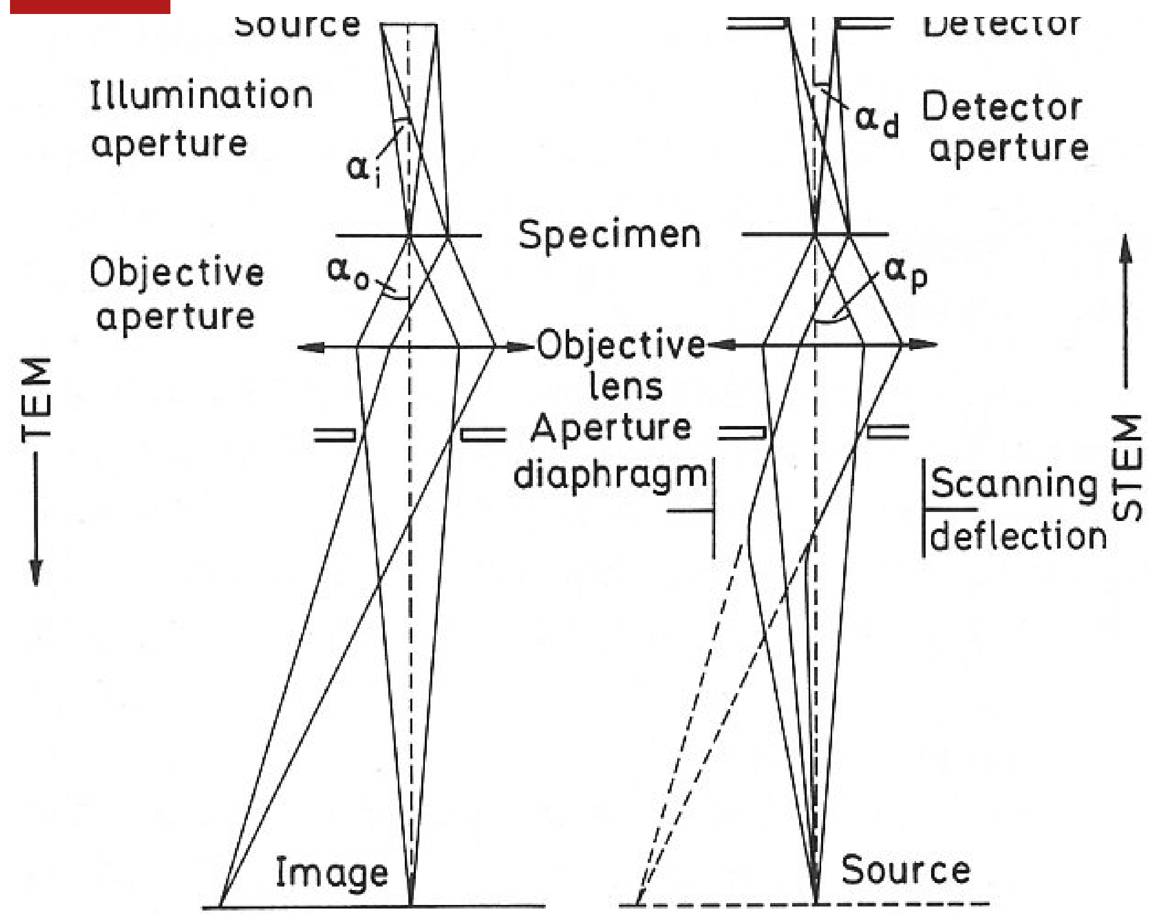
Proof follows from time-reversal symmetry of the electron trajectories and elastic scattering (to all orders).

Reciprocity does not hold for inelastic scattering:
Sample is after probe forming optics in STEM - energy losses in sample do not cause chromatic blurring in the image

Sample is before the imaging optics in TEM – energy losses in the sample do cause chromatic blurring in the image. Imaging thick samples in TEM can be improved by energy filtering (so on the zero-loss image is recorded). This is not needed for STEM.

From L. Reimer, *Transmission Electron Microscopy*

Reciprocity



TEM	STEM
Condensor aperture	Collector aperture
Controls coherence	
Objective aperture (after sample)	Condensor aperture (before sample)
Controls resolution	

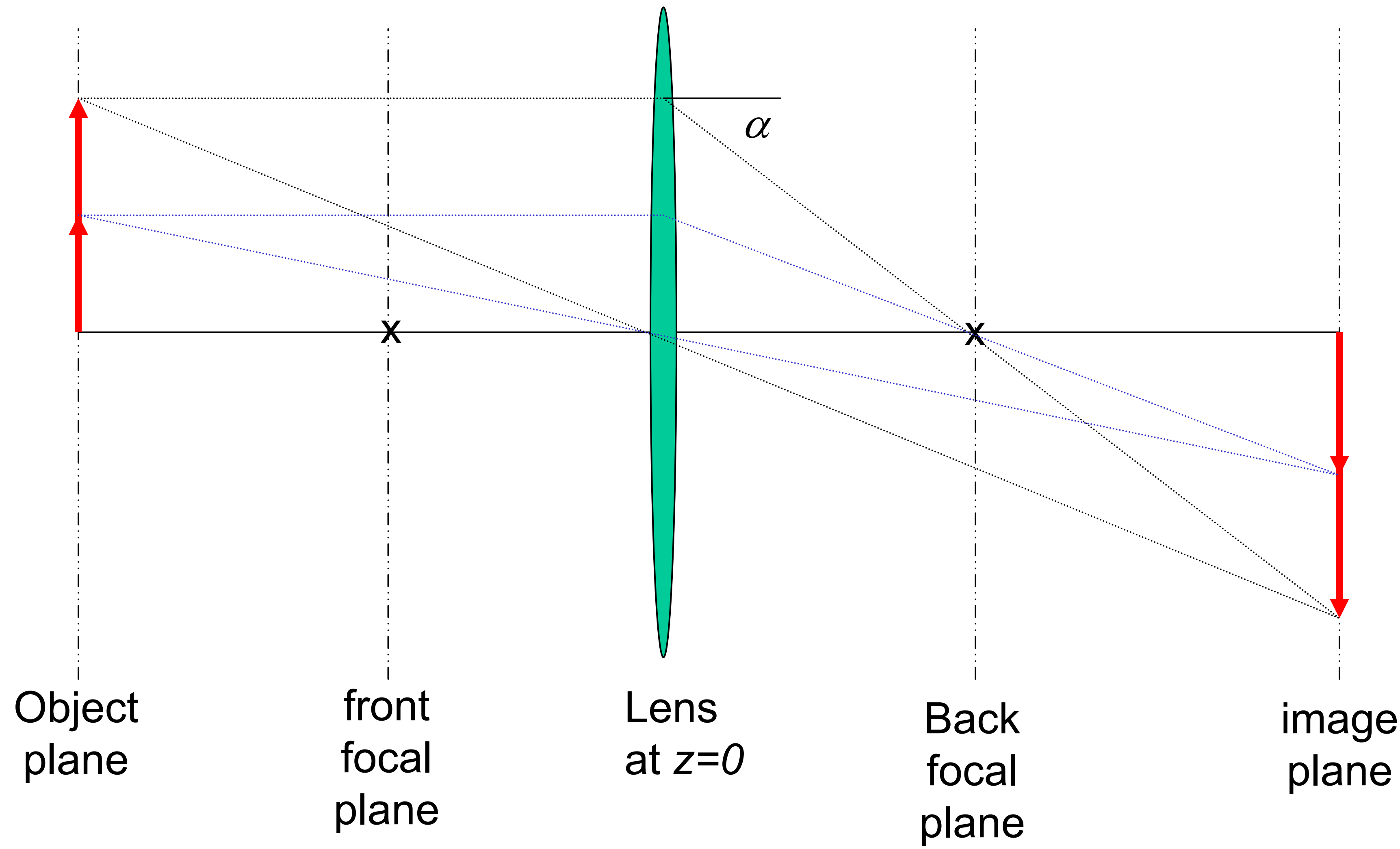
Image recorded In parallel

Image recorded serially by scanning the source

From L. Reimer, *Transmission Electron Microscopy*

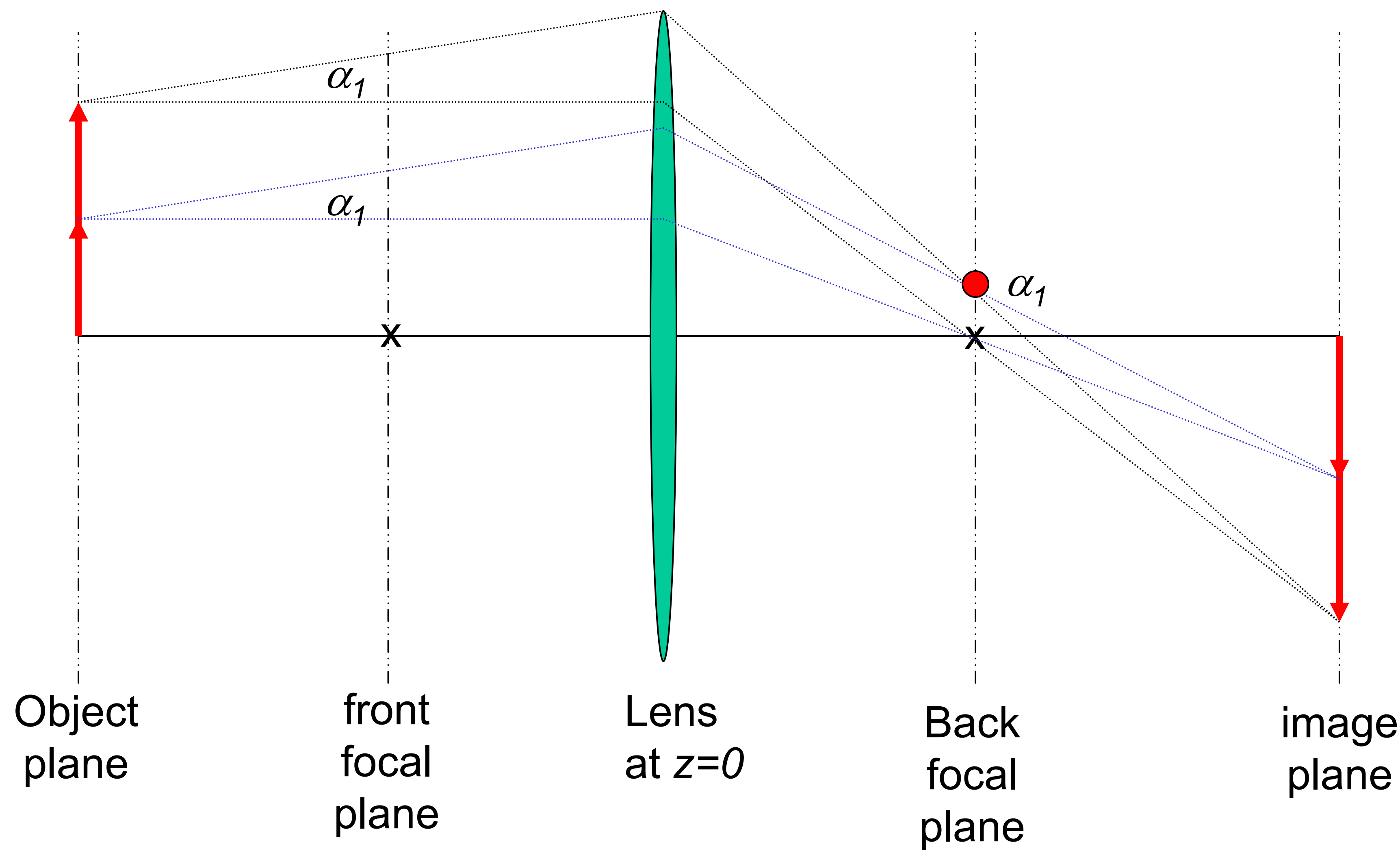
Geometric Optics – A Simple Lens

Focusing: angular deflection of ray α distance from optic axis

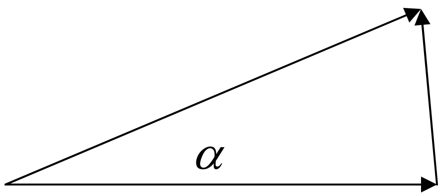


Geometric Optics – A Simple Lens

Wavefronts in focal plane are the Fourier Transform of the Image/Object



Fourier Transforms



$$k_0 = \frac{1}{\lambda}$$

$$\vec{k} \approx \frac{\vec{\alpha}}{\lambda}$$

All plane waves at angle α pass through the same point In the focal plane.

If the component of the wavevector in the focal plane is $\vec{k}$,then a function in the back focal plane, ***F(k)*** *is the Fourier transform of a function in the image plane* ***f(x)***

Forward Transform: (image- > diffraction)

$$F(\vec{k}) = \mathcal{F}\left\{f(\vec{x})\right\} = \int_{-\infty}^{\infty} f(\vec{x})\, e^{i2\pi \vec{k}.\vec{x}}\, d^2\vec{x}$$

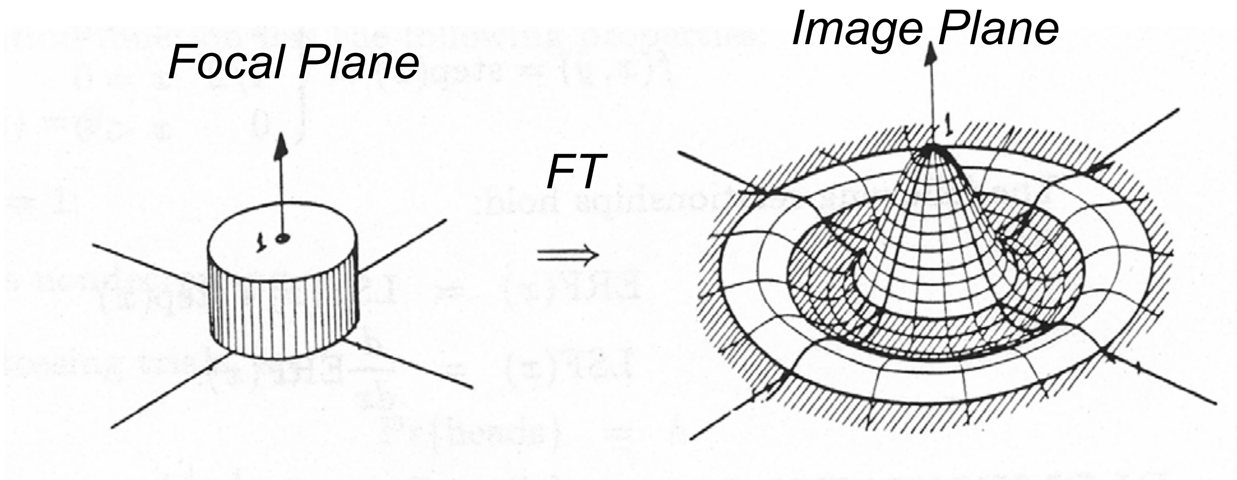
Inverse Transform: (diffraction ->image)

$$f(\vec{x}) = \mathcal{F}^{-1}\left\{F(\vec{k})\right\} = \int_{-\infty}^{\infty} F(\vec{k})\, e^{-i2\pi \vec{k}.\vec{x}}\, d\vec{s}$$

Note: in optics, we define k=1/d, while in physics k=2π/d

FT of A Circular Aperture

An ideal lens would have an aperture A(k)=1 for all k. However, there is a maximum angle that can be accepted by the lens, α_{max}, and so there is a cut-off spatial frequency $k_{max} = k_0\, \alpha_{max}$,

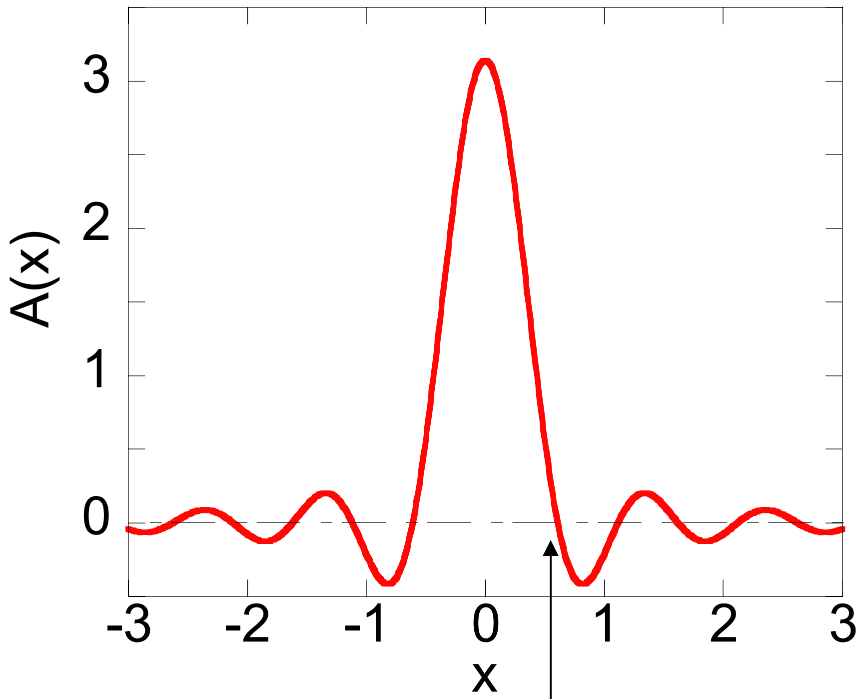


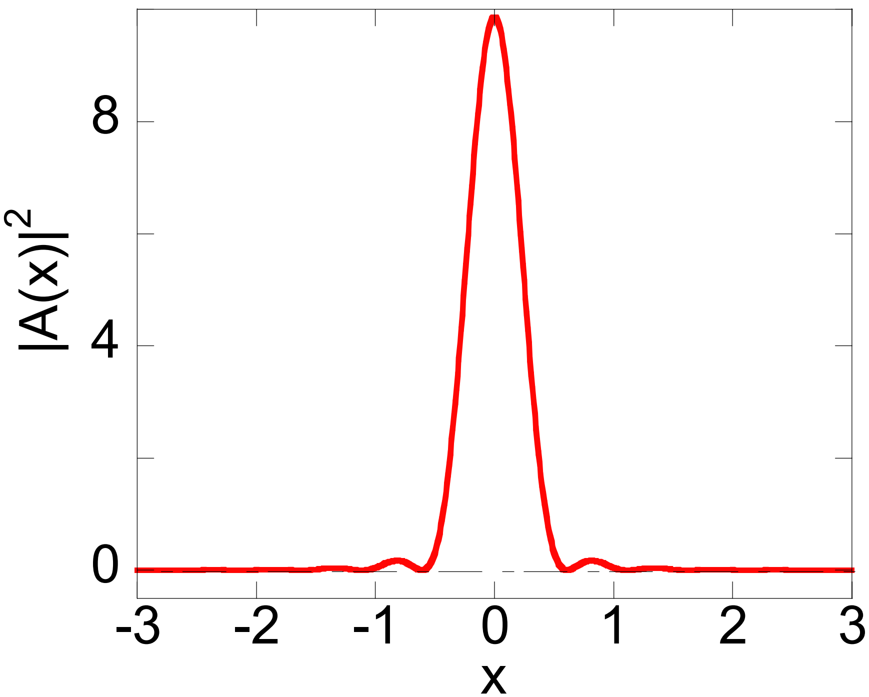
$$A(\vec{k}) = \begin{cases} 1, & |\vec{k}| < k_{\max} \\ 0, & |\vec{k}| > k_{\max} \end{cases} \qquad A(r) = \pi \frac{2 J_1(2\pi k_{\max} r)}{2\pi k_{\max} r}$$

The Aperture Function in the Image Plane

$$A(r) = \pi \frac{2J_1(2\pi k_{\max} r)}{2\pi k_{\max} r}$$

$$\left|A(r)\right|^2$$



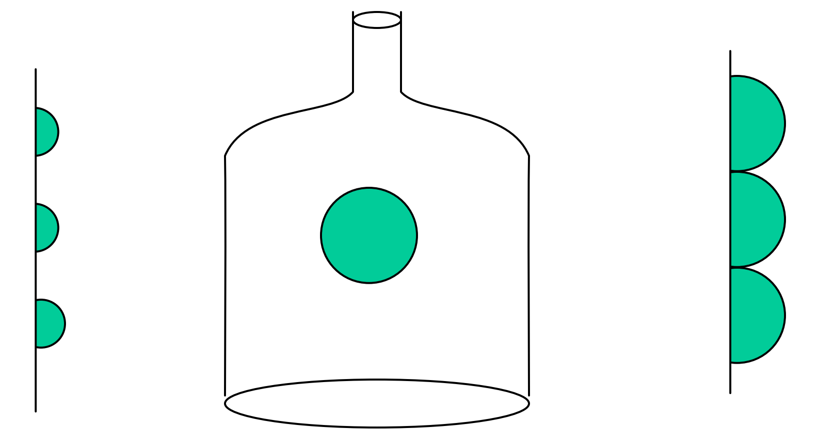


First zero at $2\pi k_{max} r = 0.61$

The image of single point becomes blurred to $\left|A(r)\right|^2$ *(why?)*

Linear Imaging *(Kirkland chapter 3)*

$$f(x) \longrightarrow \boxed{h(x)} \longrightarrow g(x)$$



object *Blurring function* *image*

Image = object convolved (symbol $\otimes$) with the blurring function, h(x)

$$g(x) = \int_{-\infty}^{\infty} f(x')\, h(x - x')\, dx' \equiv f(x) \otimes h(x)$$

Point spread function

In Fourier Space, convolution becomes multiplication (and visa-versa)

$$G(k) = F(k)H(k)$$

Contrast Transfer Function

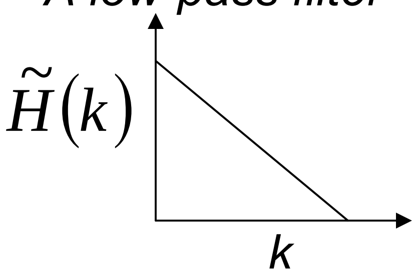
Contrast Transfer Function

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)

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

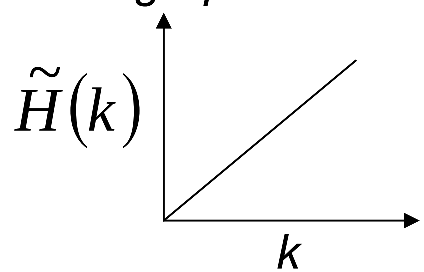
A low-pass filter



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

smoothing

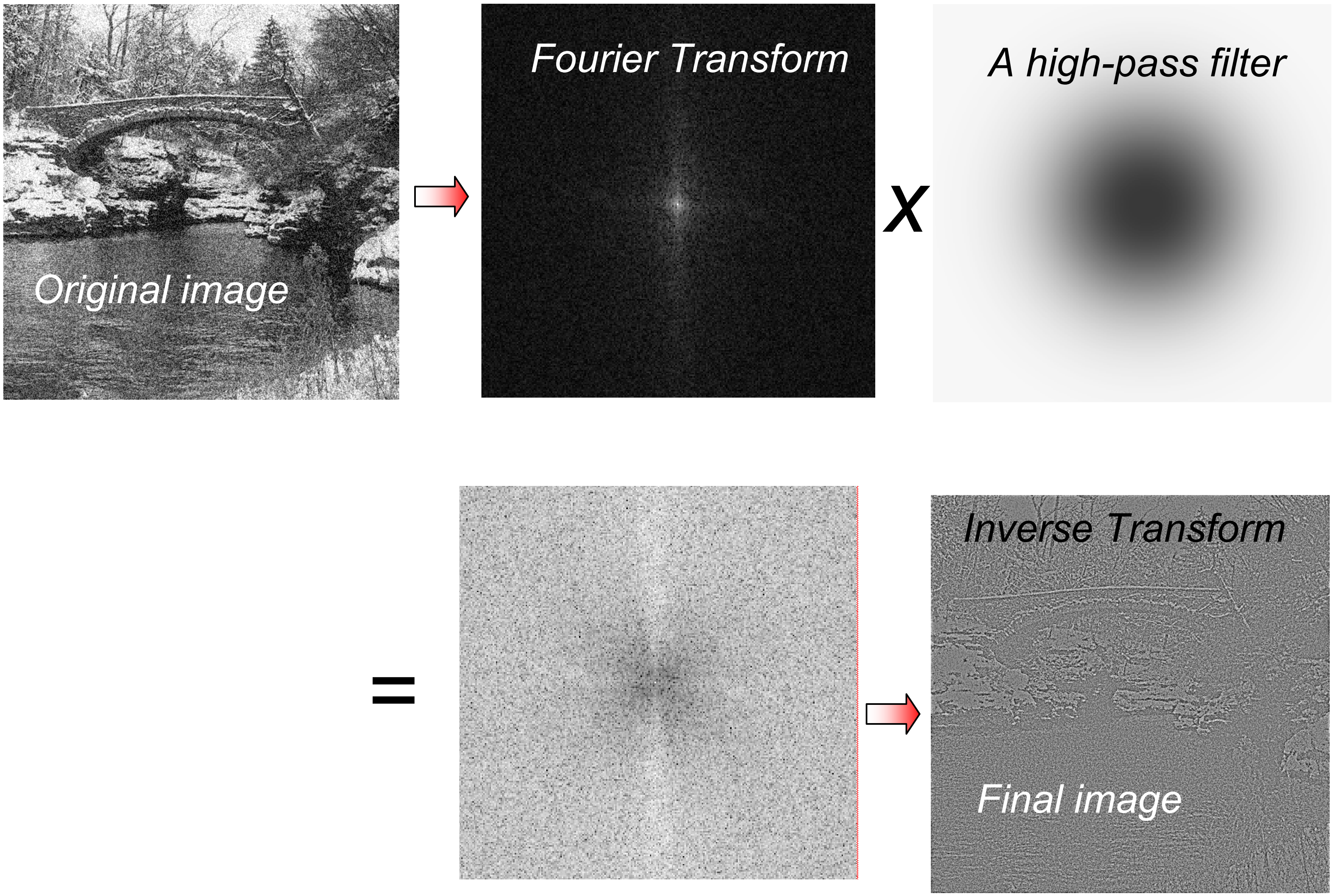
A high-pass filter



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

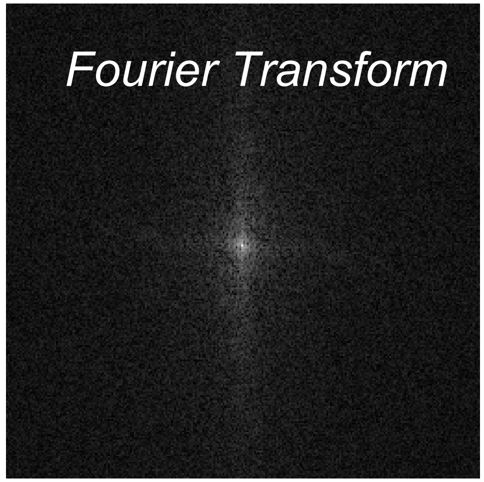
Edge-enhancing

High-pass filter

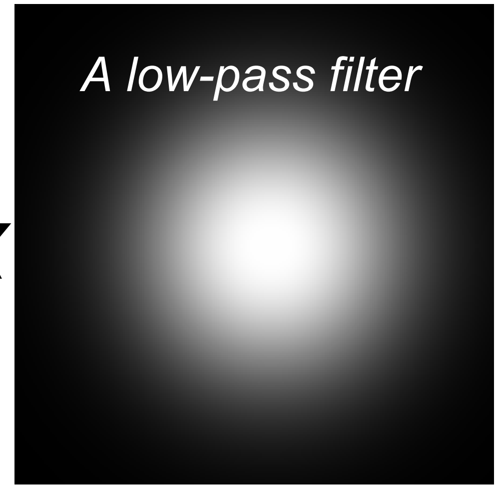


Edge-enhancing

Low pass filter



x



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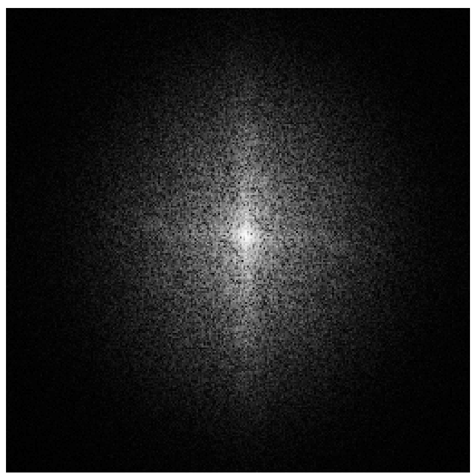
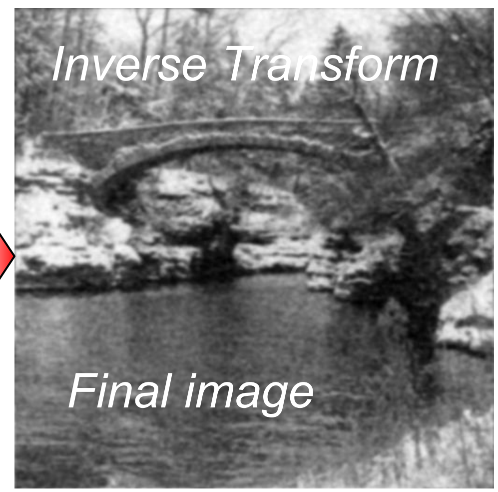




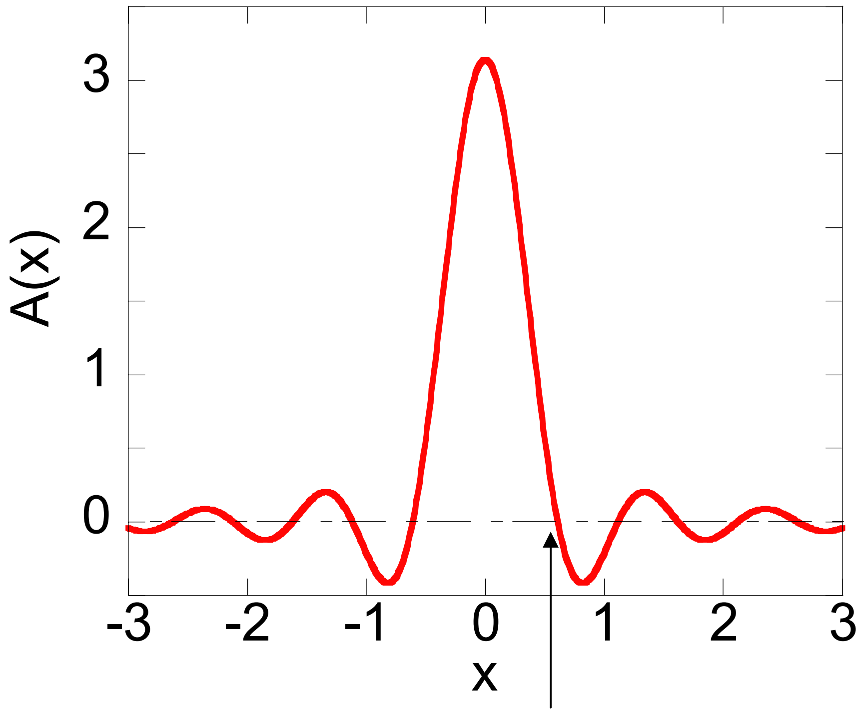
smoothing

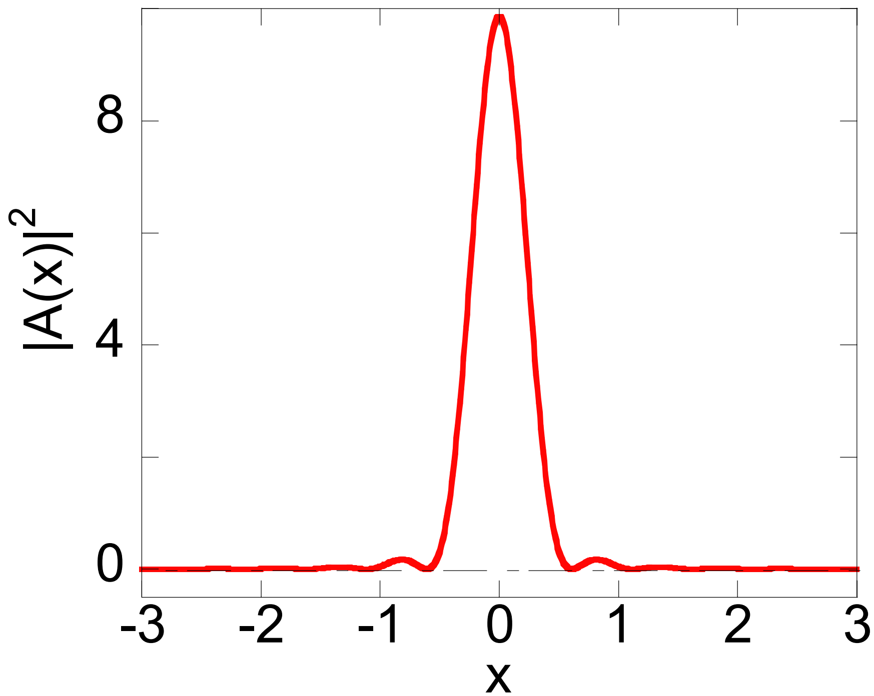
The Aperture Function in the Image Plane

The image of single point becomes blurred to $\left|A(r)\right|^2$ *(why?)*

$$A(r) = \pi \frac{2J_1(2\pi k_{max} r)}{2\pi k_{max} r}$$

$$\left|A(r)\right|^2$$

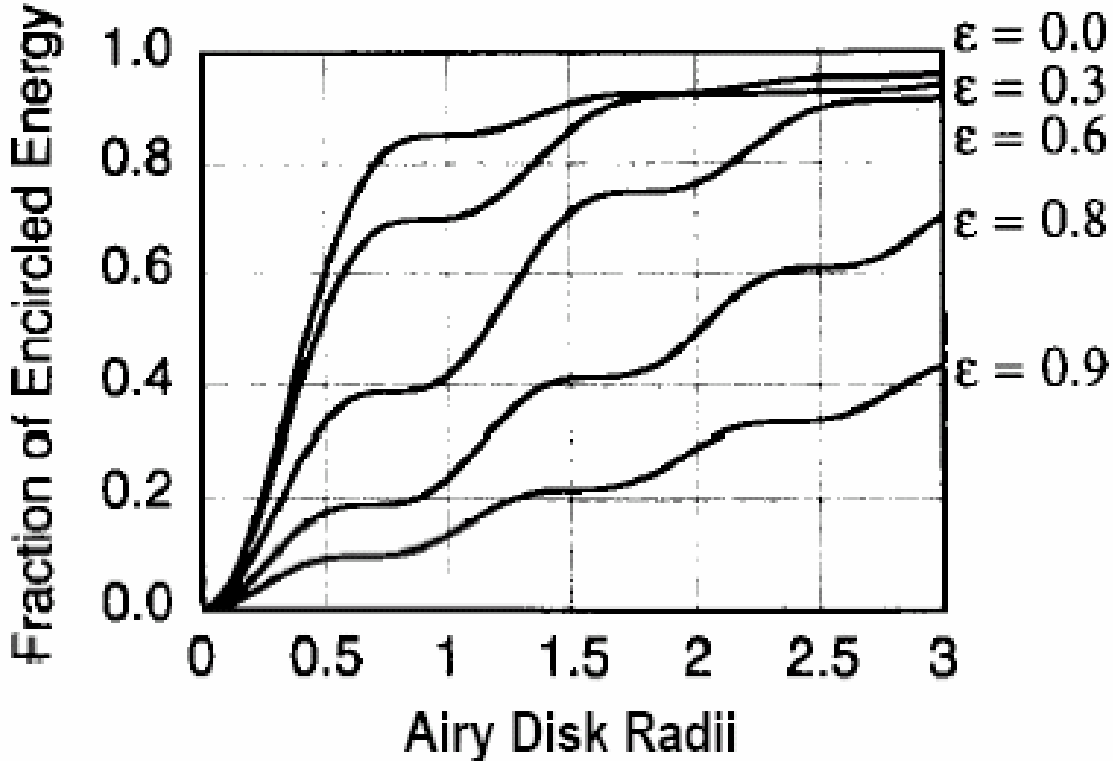


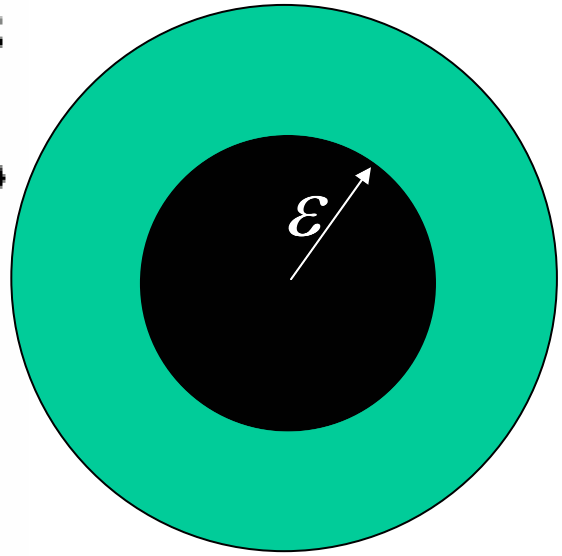


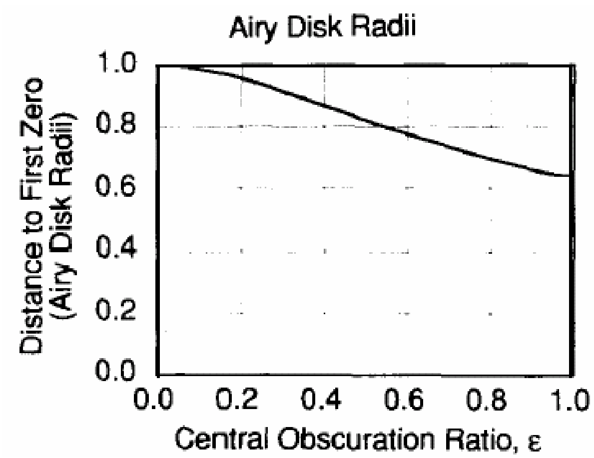
First zero at $\boldsymbol{2\pi k_{max} r = 0.61}$, ***with*** $\boldsymbol{k_{max} = (2\pi/\lambda)\theta_{max}}$

i.e. $\boldsymbol{r = 0.61/(2\pi k_{max}) \sim 0.61\ \lambda/\theta_{max}}$

Is this the best we can do?





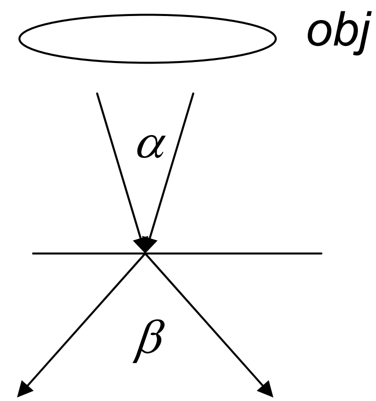


Adding a central beam-stop to the aperture increases the tails on the probe but only slighty narrows the central peak.

From Wyant and Creath

Coherent vs. Incoherent Imaging

(Kirkland, Chapter 3.3)



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

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

Combining these 2 formula we get:

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

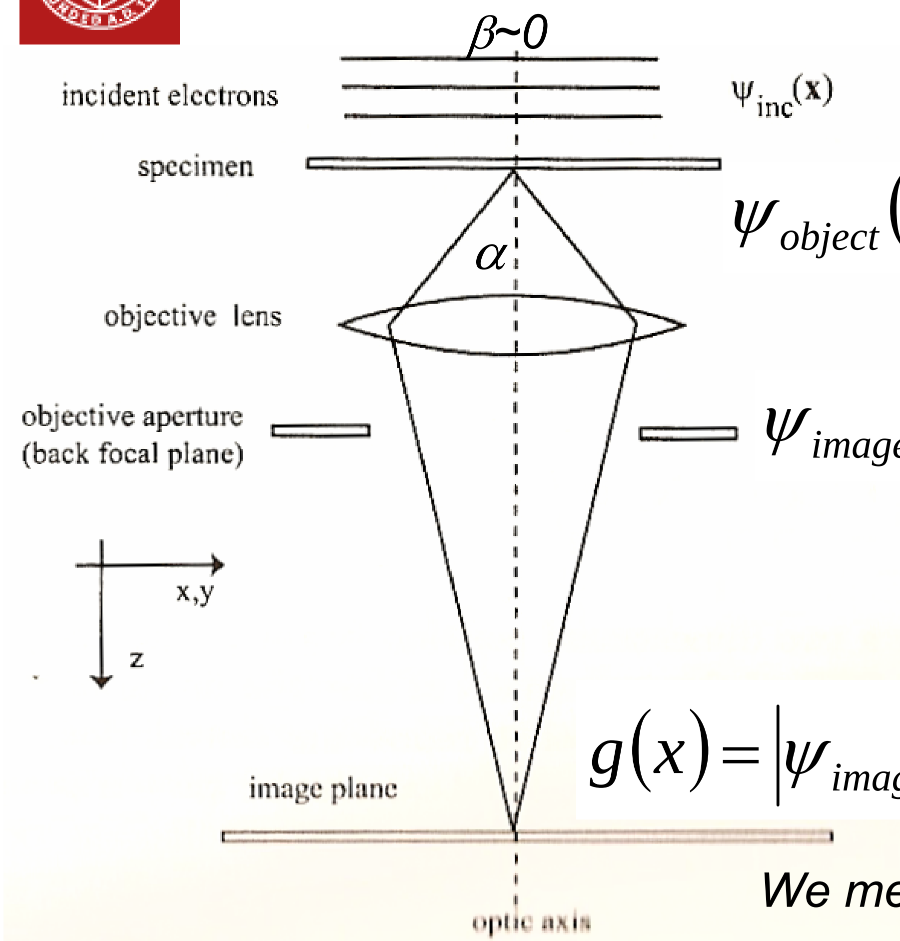
Wave Interference inside Δx_{coh} *allows us to measure phase changes as wavefunctions add:* $|\psi_a + \psi_b|^2 = |\psi_a|^2 + |\psi_b|^2 + \psi_a\psi_b^* + \psi_b\psi_a^*$

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)



Lens has a PSF A(x)

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

$$\downarrow$$

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

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

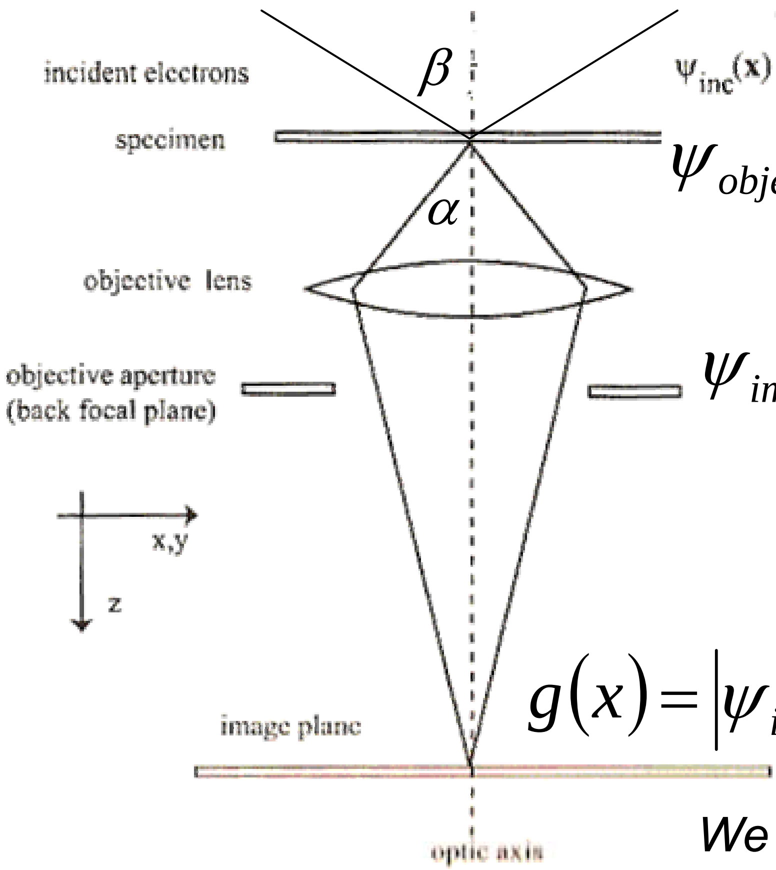
We measure the intensity, not the wavefunction

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

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 $\left|A(x)\right|^2$

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

$$\downarrow$$

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

We measure the intensity, not the wavefunction

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

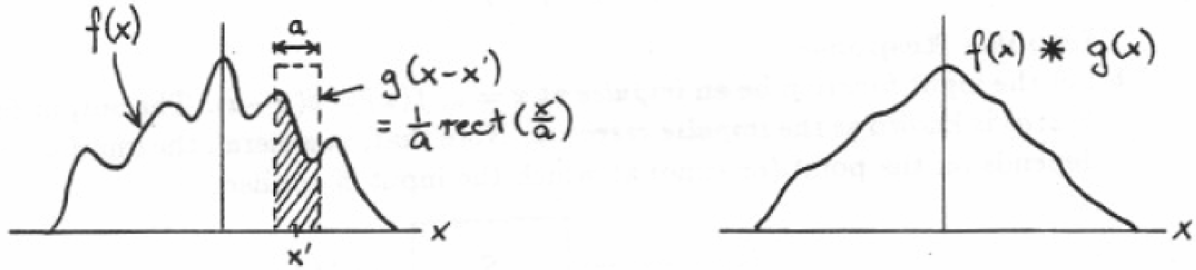
Convolve intensities, measure intensities

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

Convolutions

(from Linear Imaging Notes, Braun)

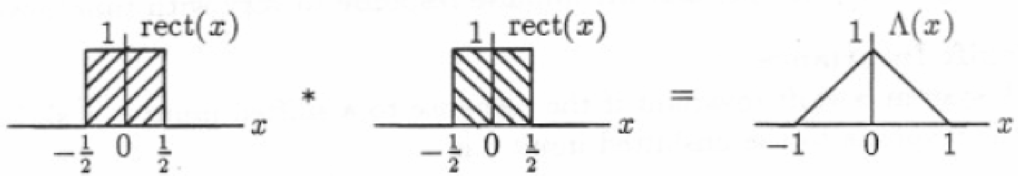


The moving average is obtained by placing the window $g(x) = (1/a)\mathrm{rect}(x/a)$ at a point $x = x'$, then computing the average within the window. The process is repeated as the window is moved to each new value of x'. The result of the moving average operation is a smoother and more spread out function. If the window function is allowed to take any form, then the moving average will generalise to a convolution.

The *graphical algorithm* for performing convolution is as follows:

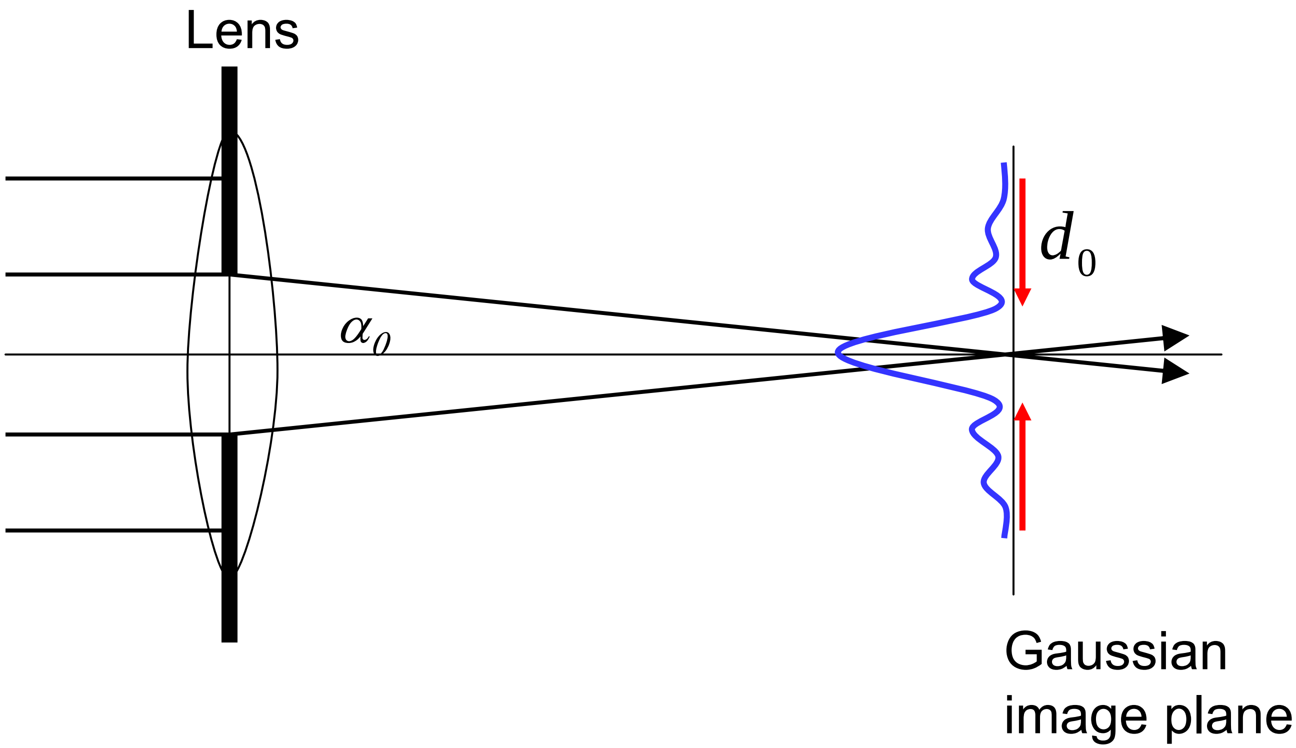
1. take $g(x')$ and flip to get $g(-x')$;
2. shift to right by x to get $g(x - x')$;
3. multiply by $f(x)$;
4. integrate the product;
5. repeat above steps for every point x.

Example: $h(x) = \mathrm{rect}(x) * \mathrm{rect}(x)$. The result of convolving a rectangle function with itself is a triangle function:



Resolution Limits Imposed by the Diffraction Limit

(Less diffraction with a large aperture – must be balanced against C_s)

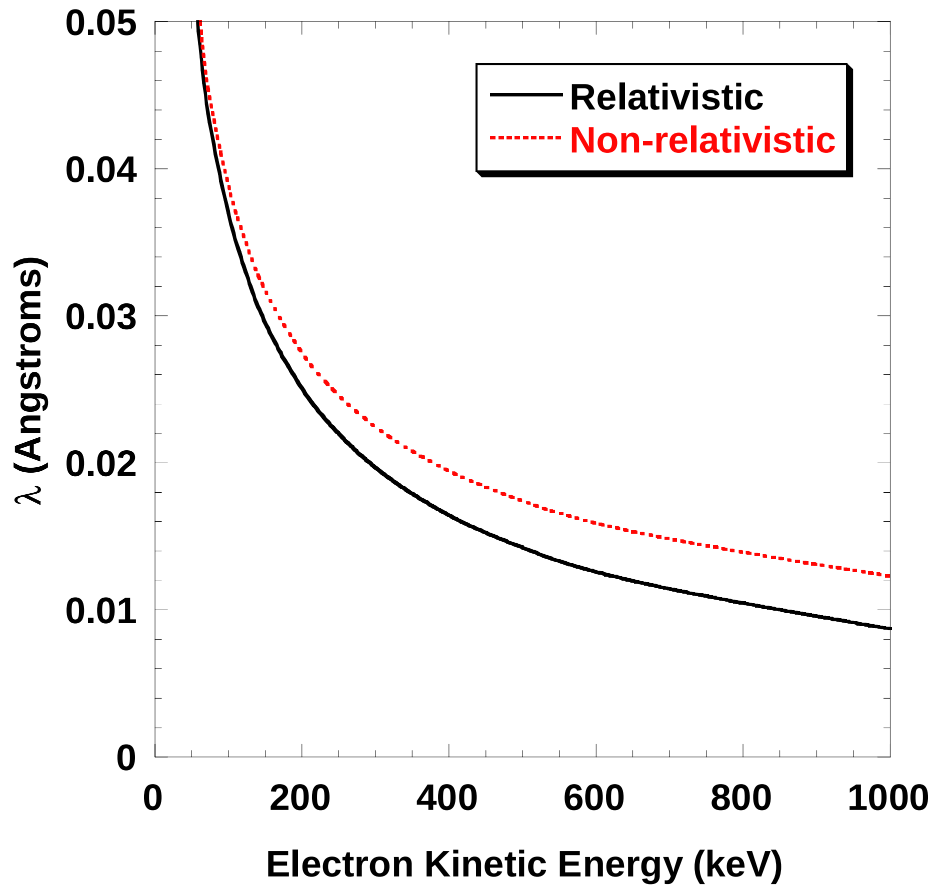


The image of a point transferred through a lens with a circular aperture of semiangle α_0 is an Airy disk of diameter $d_0 = \dfrac{0.61\lambda}{n \sin \alpha_0} \approx \dfrac{0.61\lambda}{\alpha_0}$

(0.61 for incoherent imaging e.g. ADF-STEM, 1.22 for coherent or phase contrast,. E.g TEM)

(for electrons, n~1, and the angles are small)

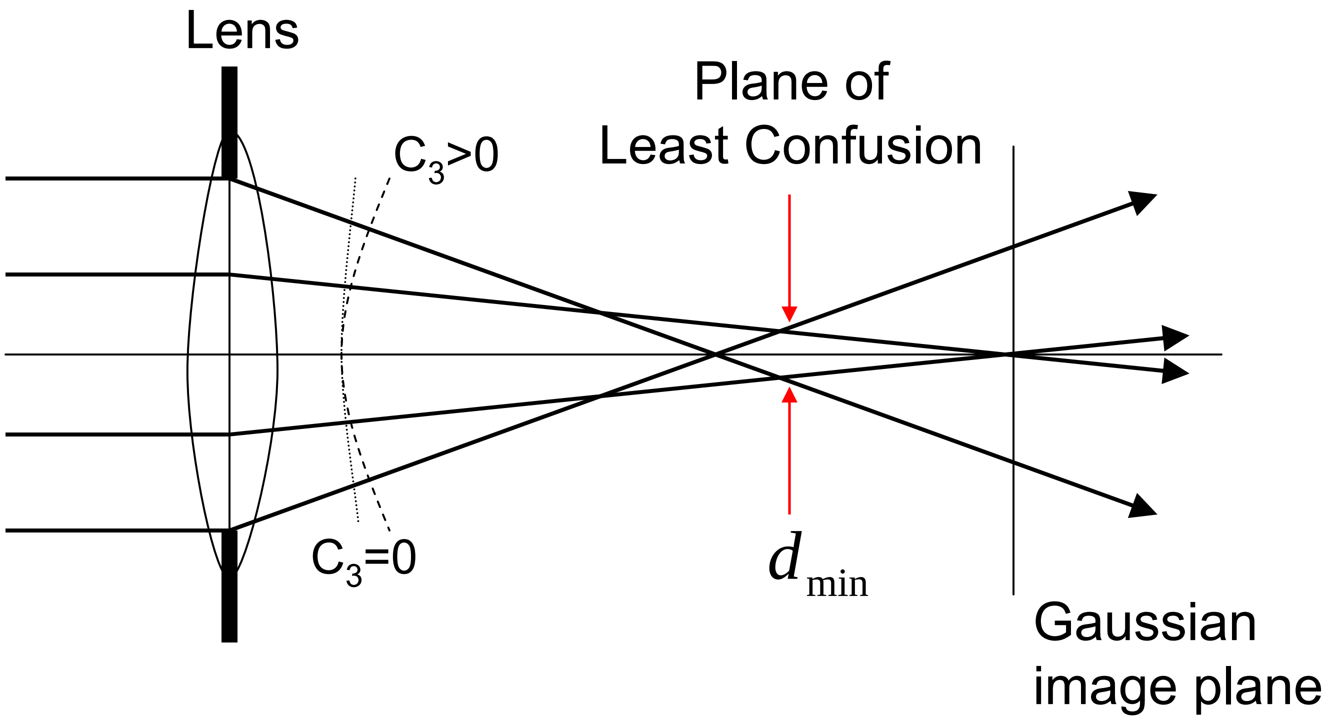
Electron Wavelength vs. Accelerating Voltage



Accelerating Voltage	*v/c*	*λ (Å)*
1 V	*0.0019784*	*12.264*
100 V	*0.0062560*	*1.2263*
1 keV	*0.062469*	*0.38763*
10 keV	*0.019194*	*0.12204*
100 keV	*0.54822*	*0.037013*
200 keV	*0.69531*	*0.025078*
300 keV	*0.77653*	*0.019687*
1 MeV	*0.81352*	*0.0087189*

Resolution Limits Imposed by Spherical Aberration, C_3

(Or why we can't do subatomic imaging with a 100 keV electron)



For C_s>0, rays far from the axis are bent too strongly and come to a crossover before the gaussian image plane.

For a lens with aperture angle α, the minimum blur is $d_{min} = \frac{1}{2} C_3 \alpha^3$

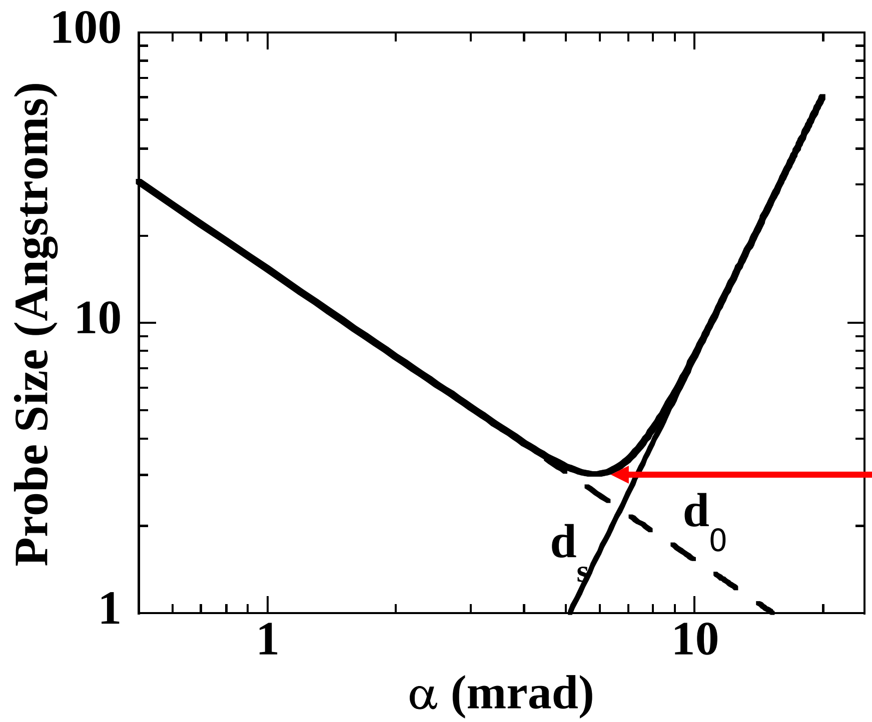
Typical TEM numbers: C_3= 1 mm, α=10 mrad $\rightarrow$ d_{min}= 0.5 nm

Balancing Spherical Aberration against the Diffraction Limit

(Less diffraction with a large aperture – must be balanced against C_s)

For a rough estimate of the optimum aperture size, convolve blurring terms
-If the point spreads were gaussian, we could add in quadrature:

$$d_{tot}^2 \approx d_0^2 + d_s^2 = \left(\frac{0.61\lambda}{\alpha_0}\right)^2 + \left(\frac{1}{2}C_3\alpha_0^3\right)^2$$



Optimal aperture
And minimum
Spot size

$$d_{\min} = 0.66 C_3^{1/4}\lambda^{3/4}$$

Balancing Spherical Aberration against the Diffraction Limit

(Less diffraction with a large aperture – must be balanced against C_3)

A more accurate wave-optical treatment, allowing less than $\lambda/4$ of phase shift across the lens gives

Minimum Spot size: $$d_{\min} = 0.43 C_3^{1/4} \lambda^{3/4}$$

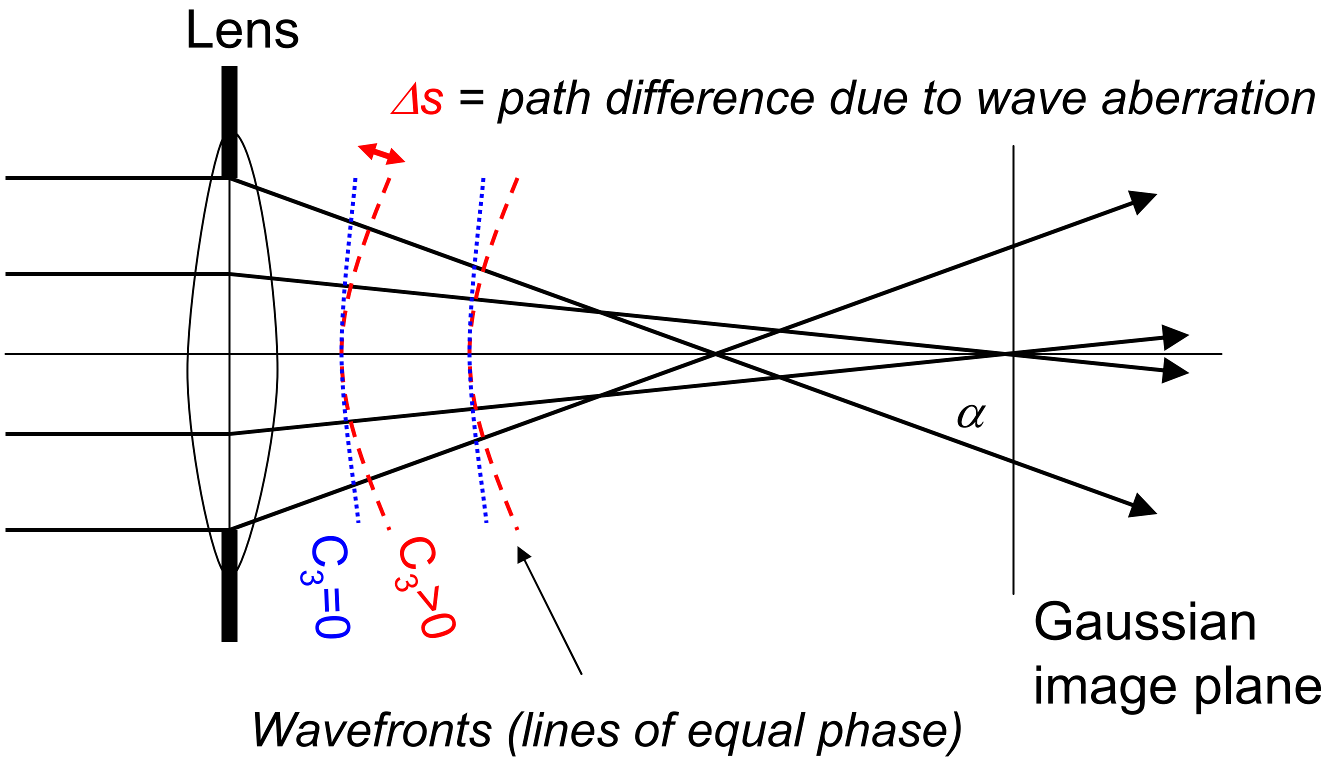
Optimal aperture: $$\alpha_{opt} = \left(\frac{4\lambda}{C_3} \right)^{1/4}$$

At 200 kV, λ=0.0257 Å, d_{min} = 1.53Å and α_{opt} = 10 mrad

At 1 kV, λ=0.38 Å, d_{min} = 12 Å and α_{opt} = 20 mrad

We will now derive the wave-optical case

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*

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

(Either Zernike Polynomials or Seidel aberration coefficients)

Zernike Polynomials

$$\chi(\rho,\theta') = Z_0 - Z_3 + Z_8 \qquad \text{piston}$$

$$+\rho\sqrt{(Z_1 - 2Z_6)^2 + (Z_2 - 2Z_7)^2} \times \cos\left[\theta' - \tan^{-1}\left(\frac{Z_2 - 2Z_7}{Z_1 - 2Z_6}\right)\right] \qquad \text{tilt}$$

$$+\rho^2\left(2Z_3 - 6Z_8 \pm \sqrt{Z_4^2 + Z_5^2}\right) \qquad \text{focus}$$

$$\pm 2\rho^2\sqrt{Z_4^2 + Z_5^2}\cos^2\left[\theta' - \frac{1}{2}\tan^{-1}\left(\frac{Z_5}{Z_4}\right)\right] \qquad \text{astigmatism}$$

$$+3\rho^3\sqrt{Z_6^2 + Z_7^2}\cos\left[\theta' - \tan^{-1}\left(\frac{Z_7}{Z_6}\right)\right] \qquad \text{coma}$$

$$+6\rho^4 Z_8. \qquad \text{spherical}$$

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

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

Seidel Aberration Coefficients (Seidel 1856)

EM community notation is similar:

O.L. Krivanek et al. / Ultramicroscopy 78 (1999) 1–11

$$
\begin{aligned}
\chi(\theta_x, \theta_y) = {} & (2\pi/\lambda)\{C_1(\theta_x^2 + \theta_y^2)/2 + C_{1,2a}(\theta_x^2 - \theta_y^2)/2 \\
& + C_{1,2b}\theta_x\theta_y + C_{2,1a}\theta_x(\theta_x^2 + \theta_y^2)/3 \\
& + C_{2,1b}\theta_y(\theta_x^2 + \theta_y^2)/3 + C_{2,3a}\theta_x(\theta_x^2 - 3\theta_y^2)/3 \\
& + C_{2,3b}\theta_y(3\theta_x^2 - \theta_y^2)/3 + C_3(\theta_x^2 + \theta_y^2)^2/4 \\
& + C_{3,2a}(\theta_x^4 - \theta_y^4)/4 + C_{3,2b}\theta_x\theta_y(\theta_x^2 + \theta_y^2)/2 \\
& + C_{3,4a}(\theta_x^4 - 6\theta_x^2\theta_y^2 + \theta_y^2)/4 \\
& + C_{3,4b}(\theta_x^3\theta_y - \theta_x\theta_y^3)\}, \qquad \text{(A.1)}
\end{aligned}
$$

where $\theta_x = \theta\cos(\phi)$ and $\theta_y = \theta\sin(\phi)$.

P.E. Batson / Ultramicroscopy 96 (2003) 239–249

Coefficient	Name	Measured (nm)
C_1	Defocus	−1034
C_{12a}	Astigmatism	11.3
C_{12b}	Astigmatism	29.3
C_{21a}	Coma	218
C_{21b}	Coma	34.8
C_{23a}		−21.7
C_{23b}		−53.7
C_3	Spherical	2062
C_{32a}		23.0
C_{32b}		−4799
C_{34a}		−1233
C_{34b}		506
C_{45a}		—
C_{45b}		—

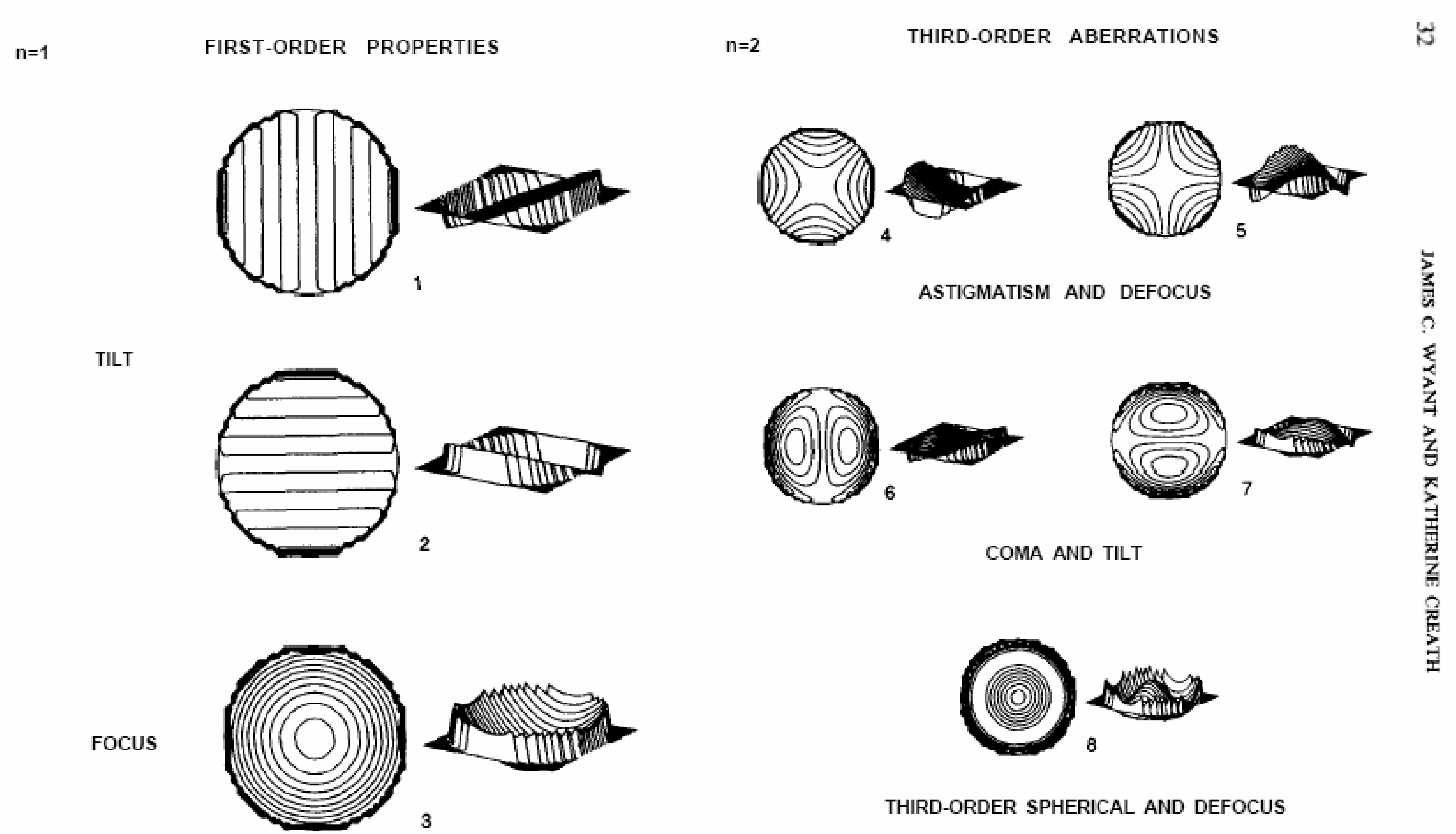
Or more generally

$$
\chi(k,\phi) = K_0 \sum_n \frac{(k/K_0)^{(n+1)}}{(n+1)} \sum_{m+n\ \mathrm{odd},\ m<n+1} \times [C_{nma}\cos(m\phi) + C_{nmb}\sin(m\phi)].
$$

$C_{5,0}$ and $C_{7,0}$ are also important

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

Here are some terms plotted out



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

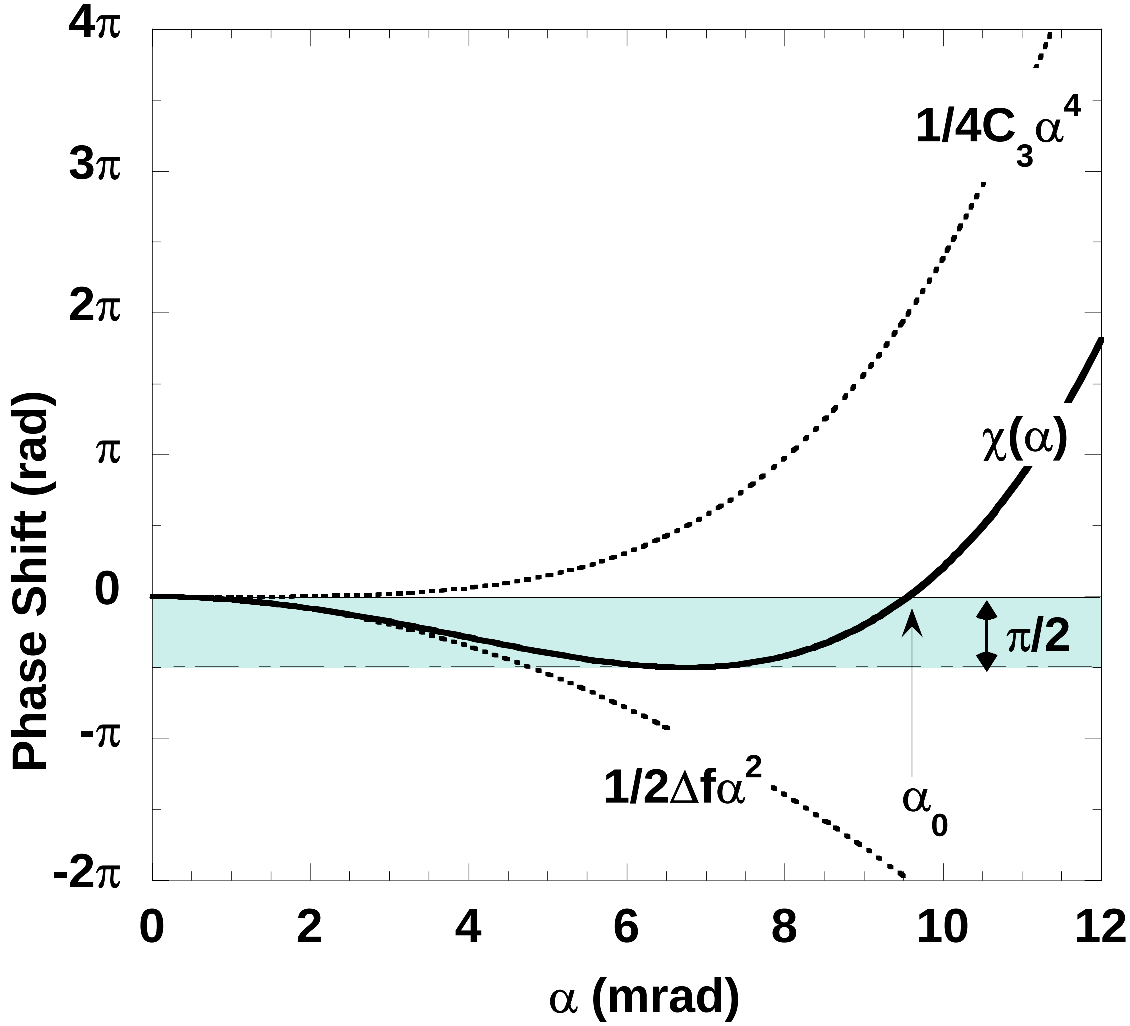
$$\chi(\alpha) = \frac{2\pi}{\lambda}\left(\frac{1}{4}C_3\alpha^4 - \frac{1}{2}\Delta f\alpha^2\right)$$

Keeping only spherical aberration and defocus

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

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 <$\lambda/4=\pi/2$ is small enough to be ignored

Step 2: Use defocus to oppose the spherical aberration shift within the widest $\pi/2$ 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 $\pi/2$ 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

Optimizing defocus and aperture size for TEM

(derivation is different, given in Kirkland 3.1)

Look for a uniform phase shift of ±π/2 across lens

Optimal defocus: $\Delta f_{opt} = \left(0.5 C_S \lambda\right)^{1/2}$

Optimal aperture: $\alpha_{opt} = \left(\dfrac{6\lambda}{C_3}\right)^{1/4}$

Minimum Spot size: $d_{\min} \approx \dfrac{1.22\lambda}{\alpha_{opt}}$

$$d_{\min} = 0.77\, C_3^{1/4} \lambda^{3/4}$$

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

Phase Shift in a Lens with an Aberration Corrector

Electron wavefunction in focal plane of the lens

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

Where the phase shift from the lens is

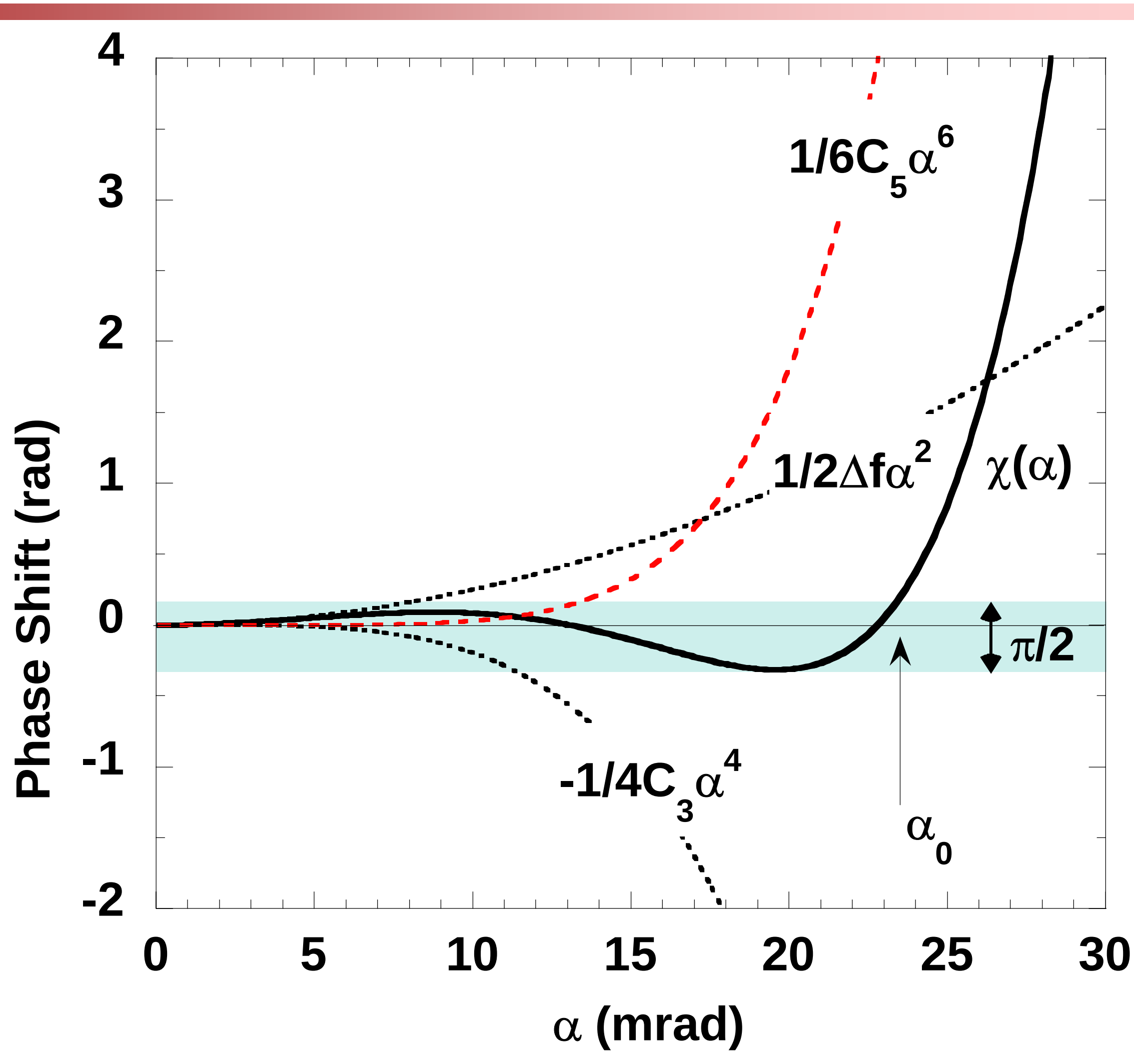
$$\chi(\alpha) = \frac{2\pi}{\lambda}\left(-\frac{1}{2}\Delta f\alpha^2 + \frac{1}{4}C_3\alpha^4 + \frac{1}{6}C_5\alpha^4 + \ldots\right)$$

5th order spherical aberration

O.L. Krivanek et al. *Ultramicroscopy* **96** (2003) 229

Optimizing Aperture size with a C_3 Corrector

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 and C_3 (now negative) to balance C_5 within the widest $\pi/2$ band

Step 3: Place aperture at upper end of the $\pi/2$ band

Optimizing defocus and aperture size

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

Step 1: We assume a phase shift <$\lambda/4=\pi/2$ is small enough to be ignored

Step 2: Use C_3 to oppose the C_5 shift within the widest $\pi/2$ band

Optimal C_3: $$C3_{opt} = -\left(3\lambda C_5^2\right)^{1/3}$$

Optimal aperture: $$\alpha_{opt} = \sqrt{\frac{3}{2}}\left(\frac{3\lambda}{C_5}\right)^{1/6} = 1.47\left(\frac{\lambda}{C_5}\right)^{1/6}$$

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

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

$$d_{\min} = 0.42\, C_5^{1/6}\,\lambda^{5/6}$$

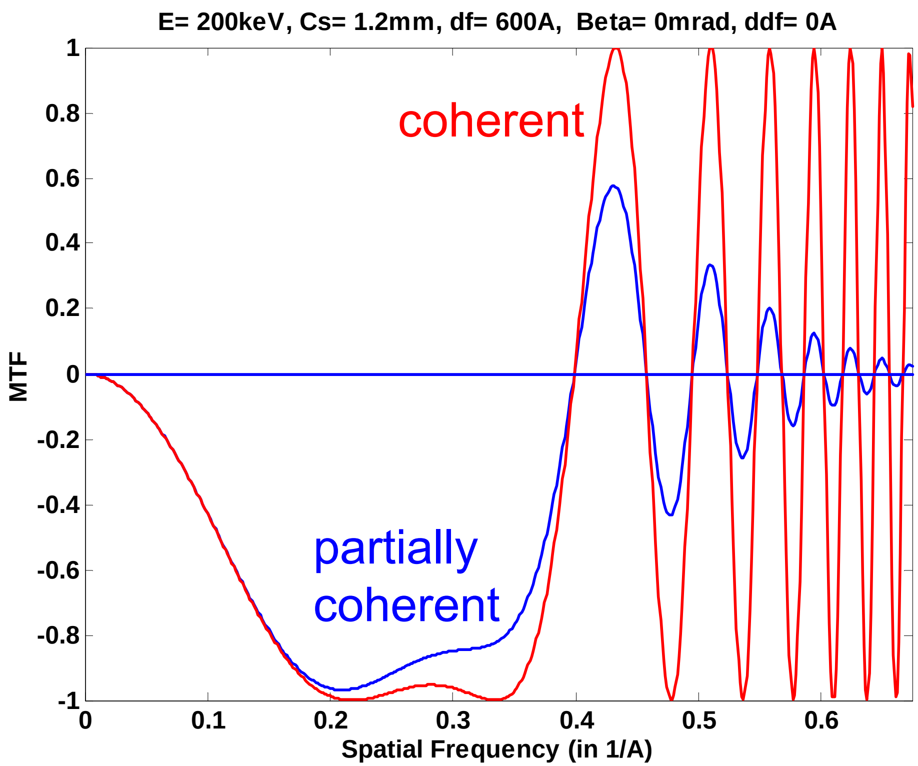
Contrast Transfer Functions of a lens with Aberrations

Generated with **`ctemtf`**

Aperture function of a real lens

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

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



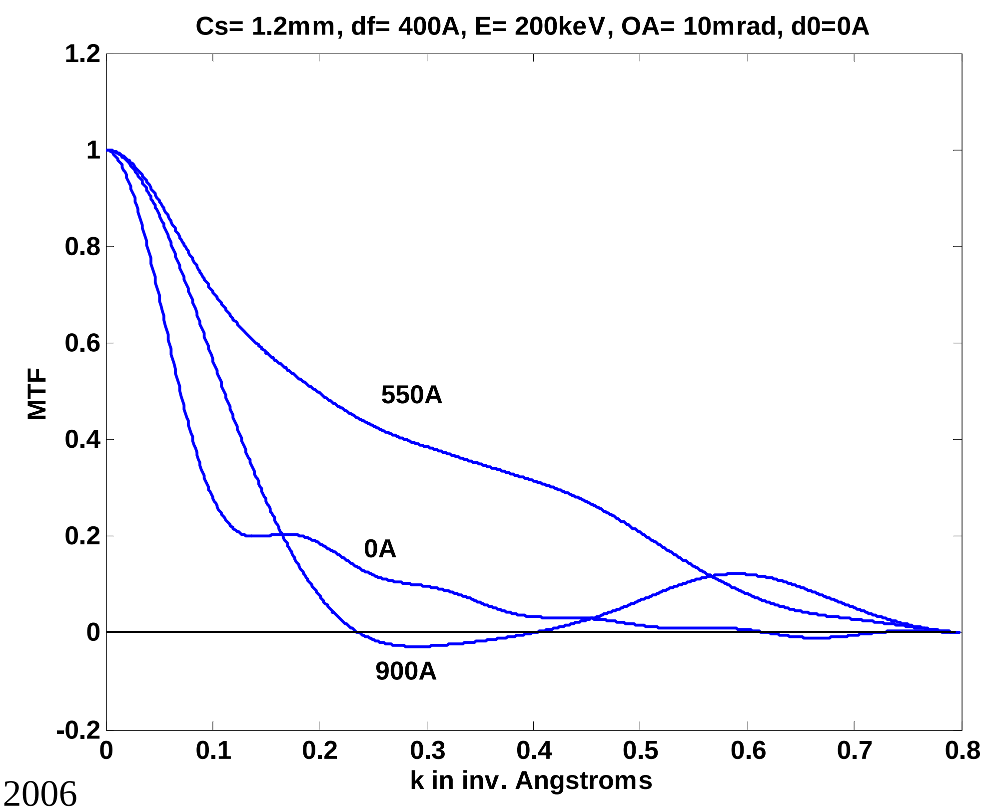
Contrast Transfer Functions of a lens with Aberrations

Generated with `stemtf`

Aperture function of a real lens

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

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

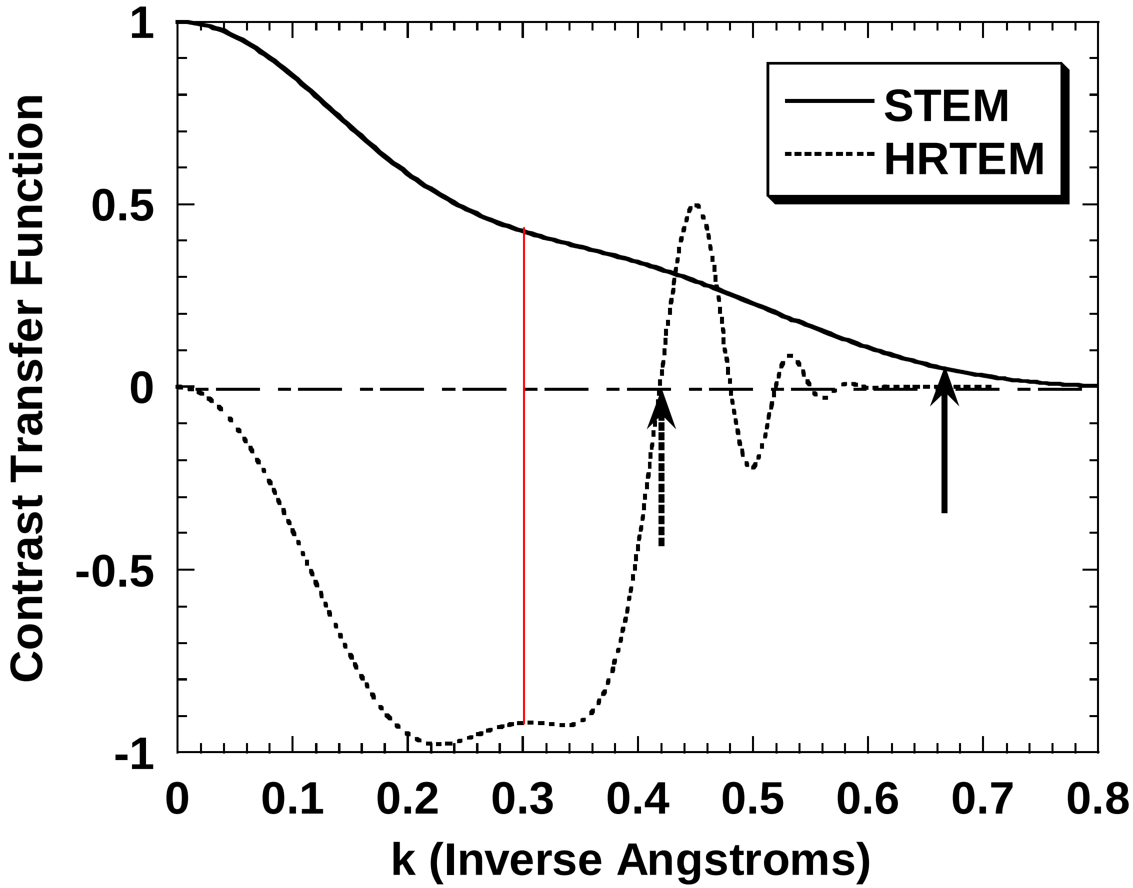


CTF for different defocii

Theorem:
Aberrations will never Increase the MTF For incoherent imaging

Phase vs. ADF Contrast

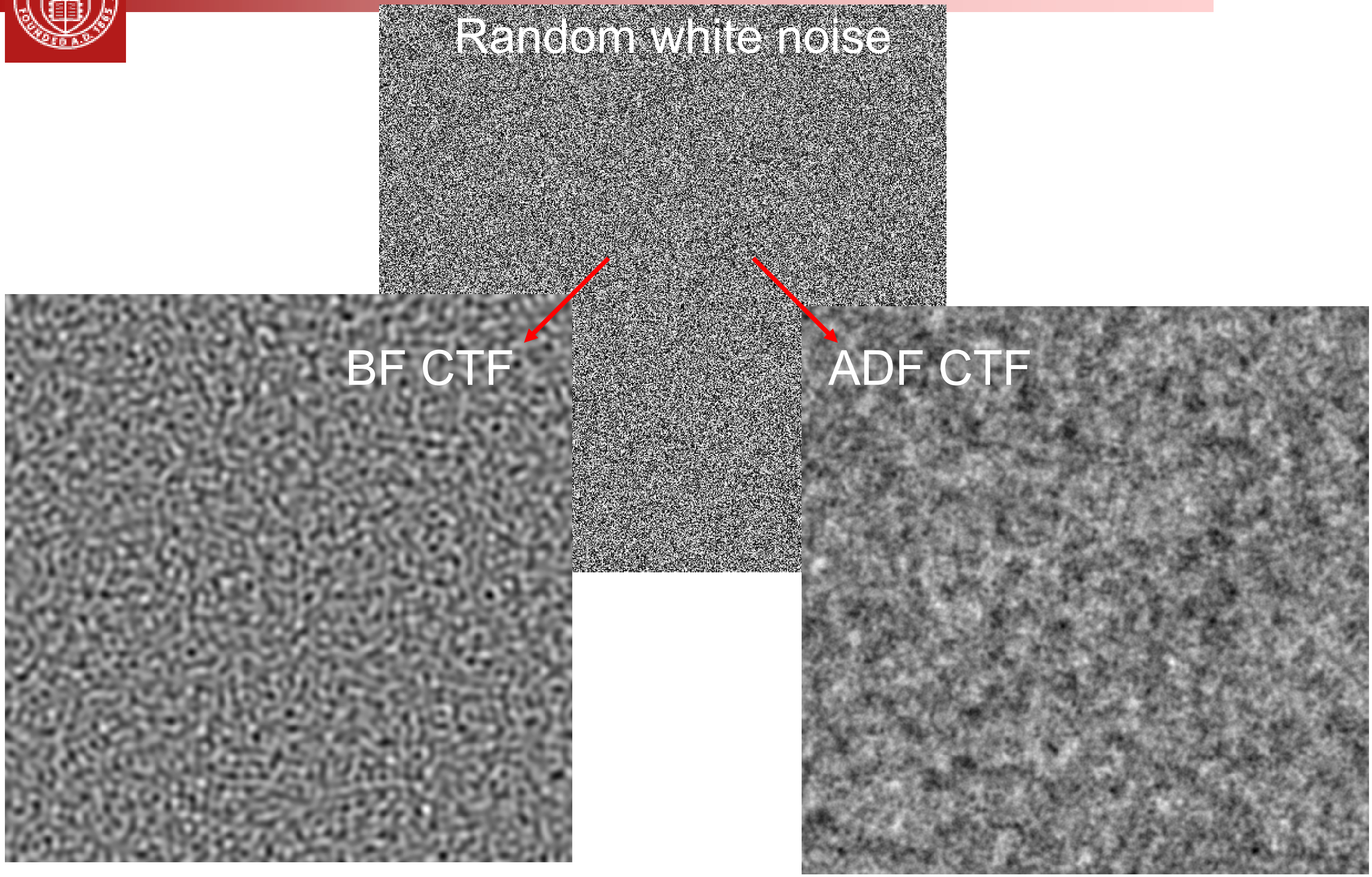
(JEOL 2010F, C_s=1mm)



TEM: Bandpass filter:low frequencies removed = artificial sharpening

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

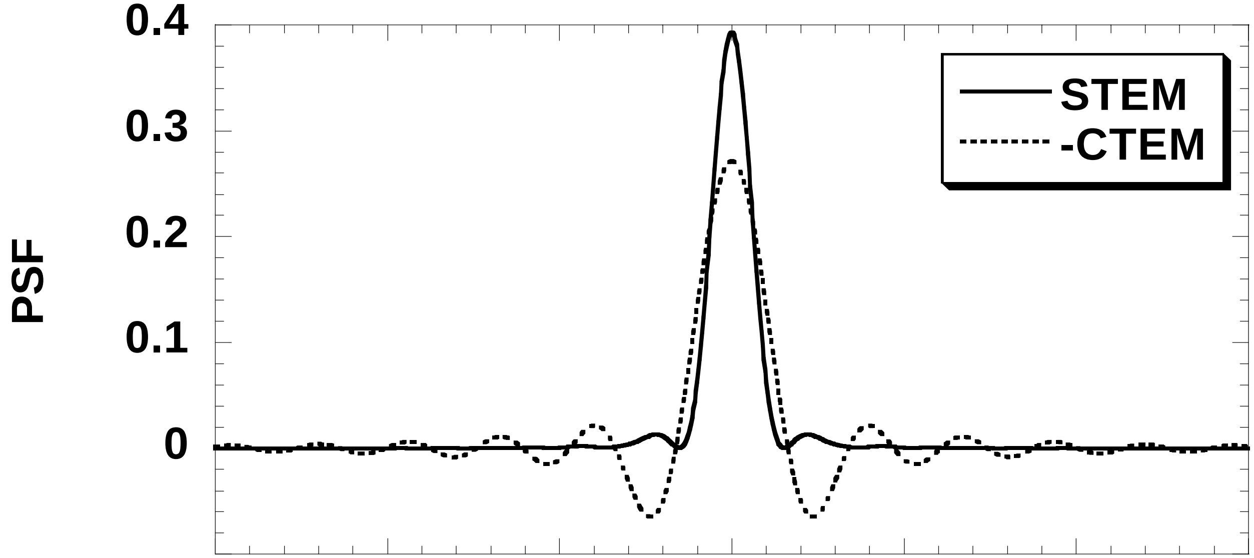
Phase vs. ADF Contrast



a-C support films look like this

Phase vs. ADF Contrast

(JEOL 2010F, C_s=1mm, Scherzer aperture and focus)



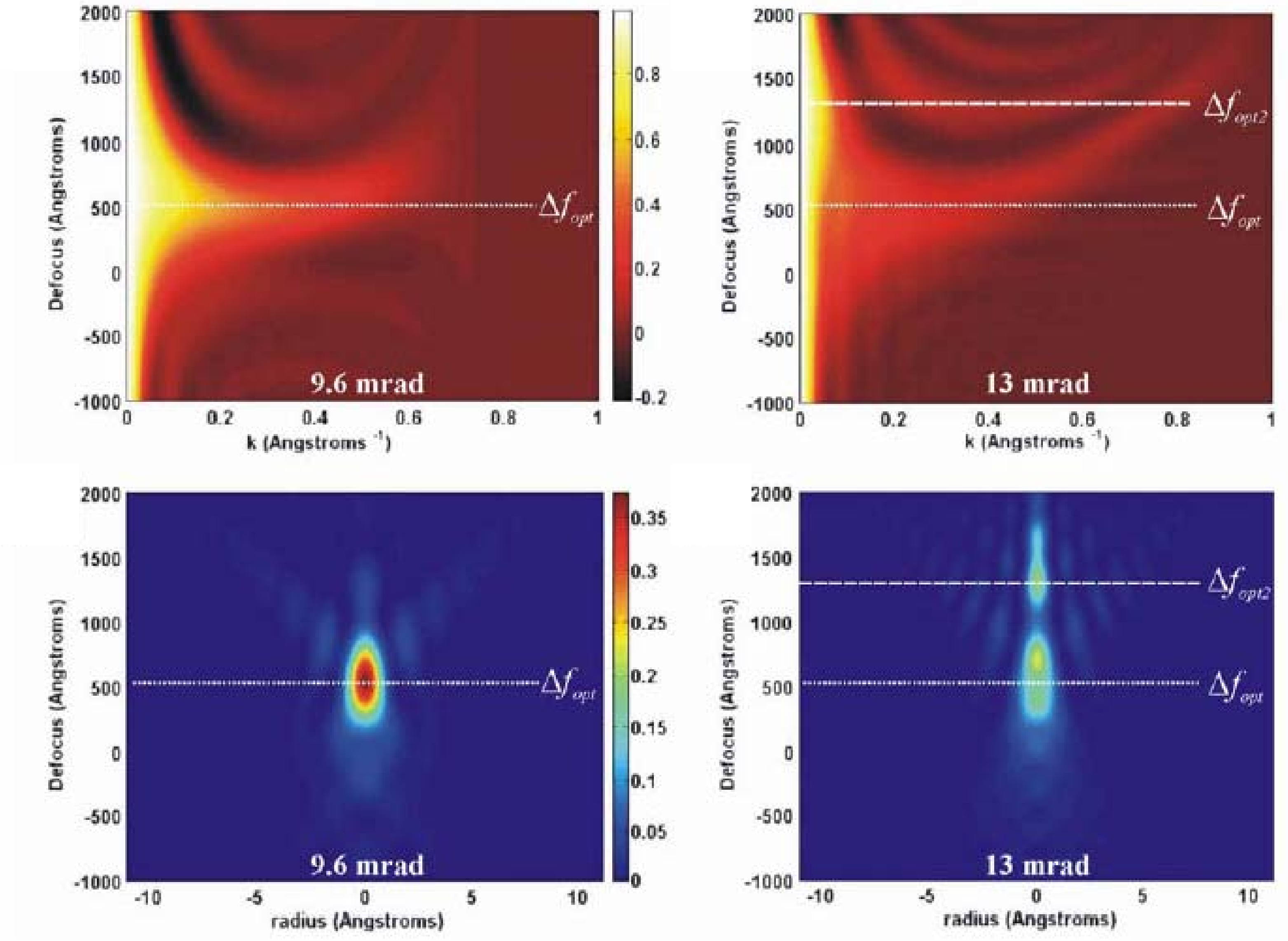
ADF : 40% narrower FWHM, smaller probe tails

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

(200 kV, C_3=1.2 mm)

CTF

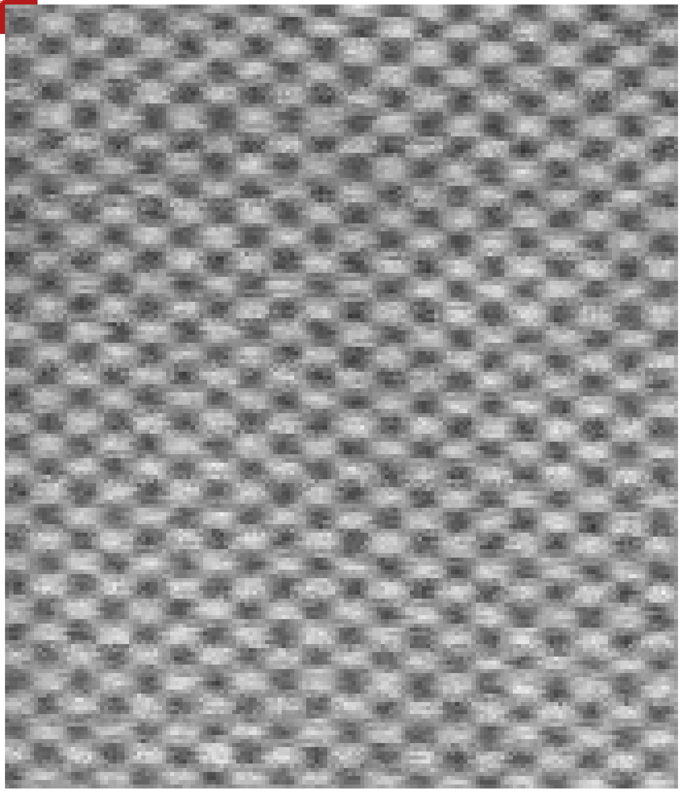
PSF



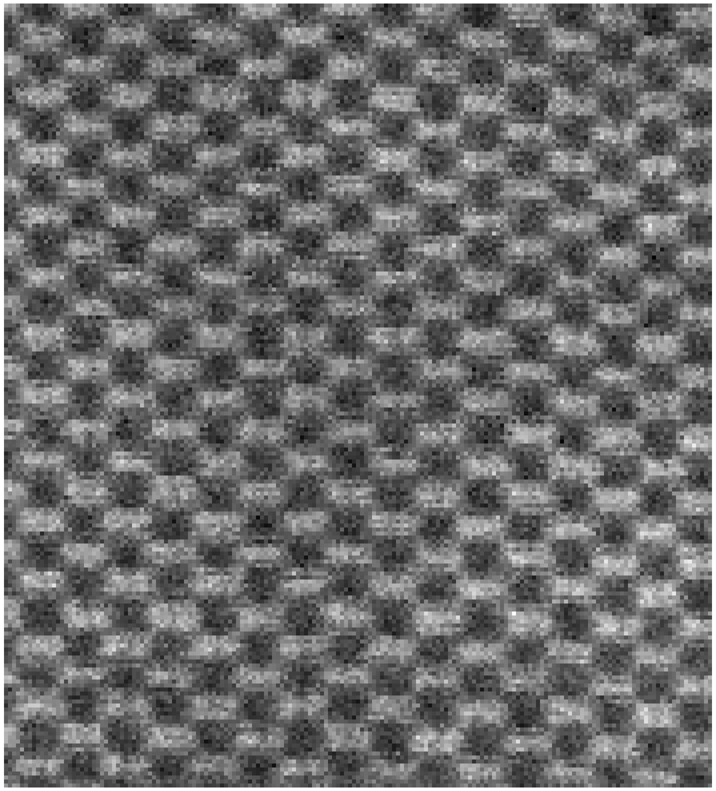
David Muller 2006

What happens with a too-large aperture?

ADF of [110] Si at 13 mr, C3=1mm



Strong {111} fringes



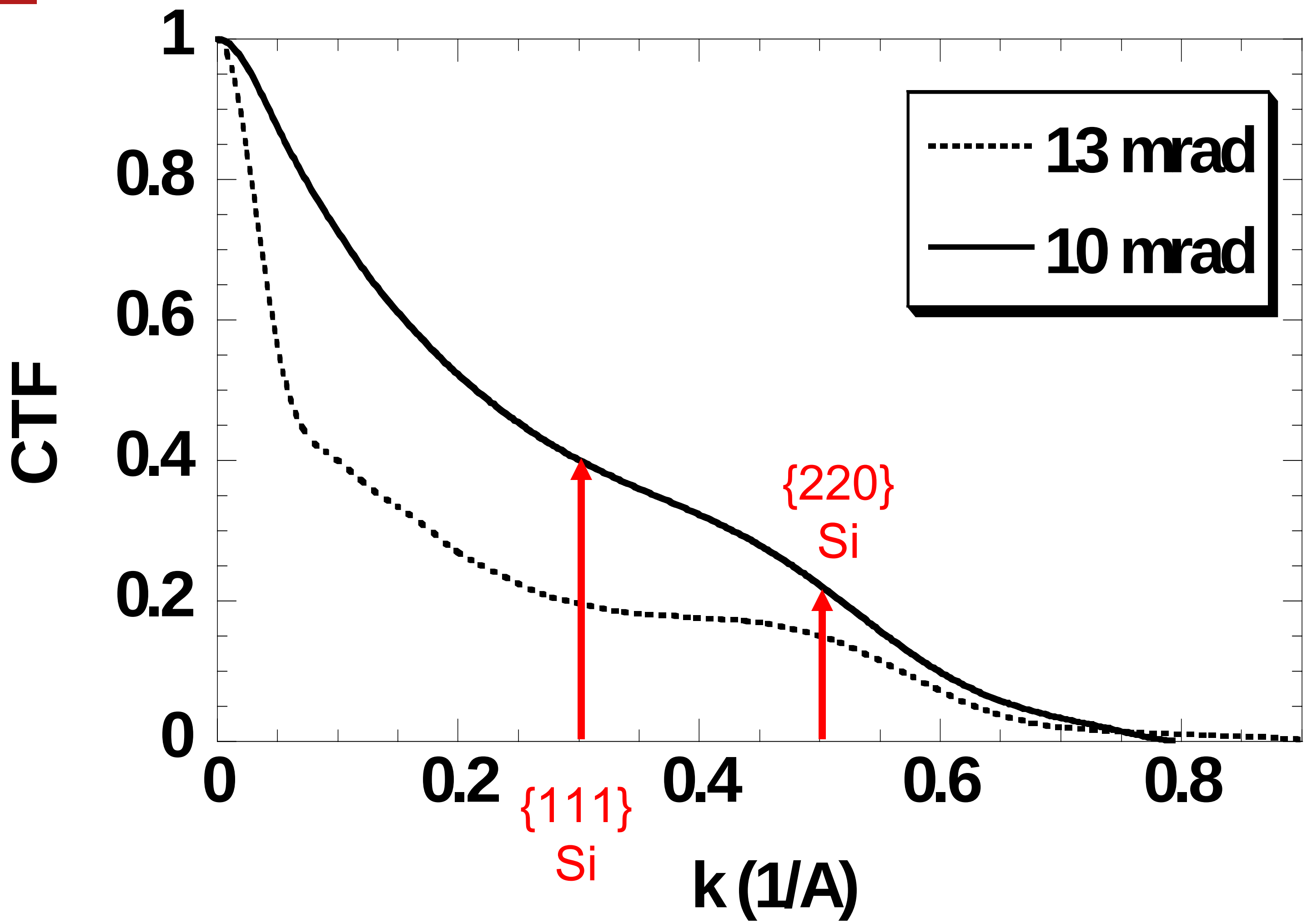
Strong {311} fringes

2 clicks overfocus

Best 111 and 311 fringes occur at different focus settings
If the aperture is too large

Aperture Size is Critical

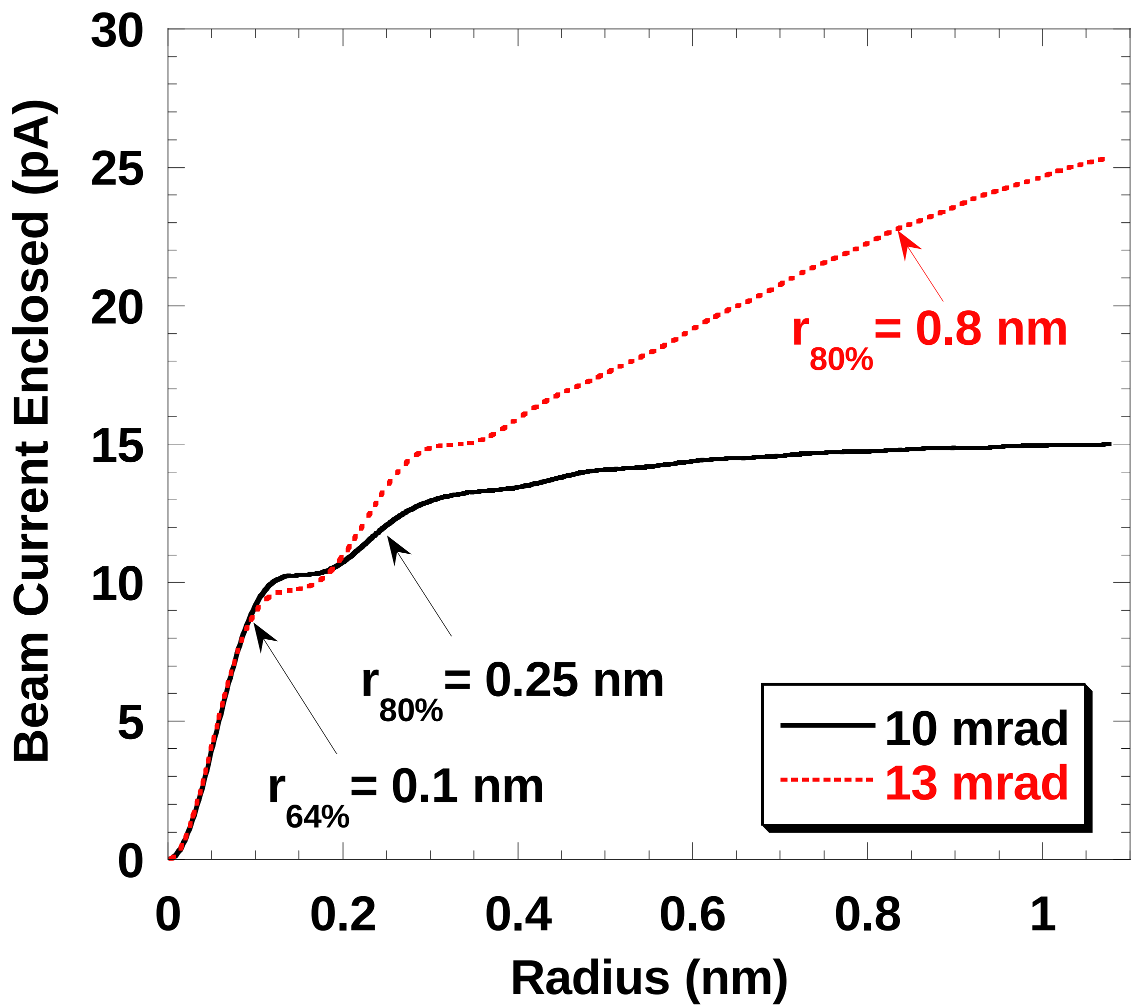
(200 kV C_3=1mm)



30% increase in aperture size ⇨ ~50% decrease in contrast for Si {111} fringes

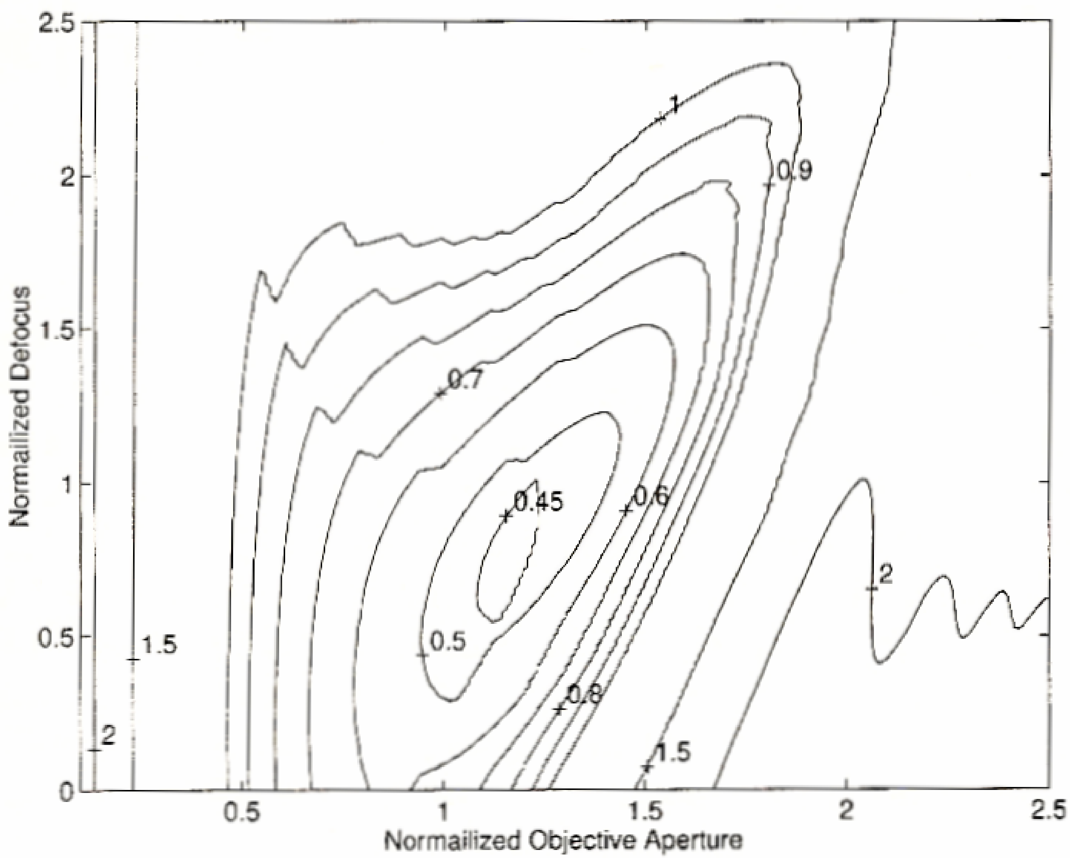
Aperture Size is Critical

(200 kV C_3=1mm)



All the extra probe current falls into the tails of the probe – reduces SNR

Finding the Aperture with the smallest probe tails (Kirkland, Fig 3.11)

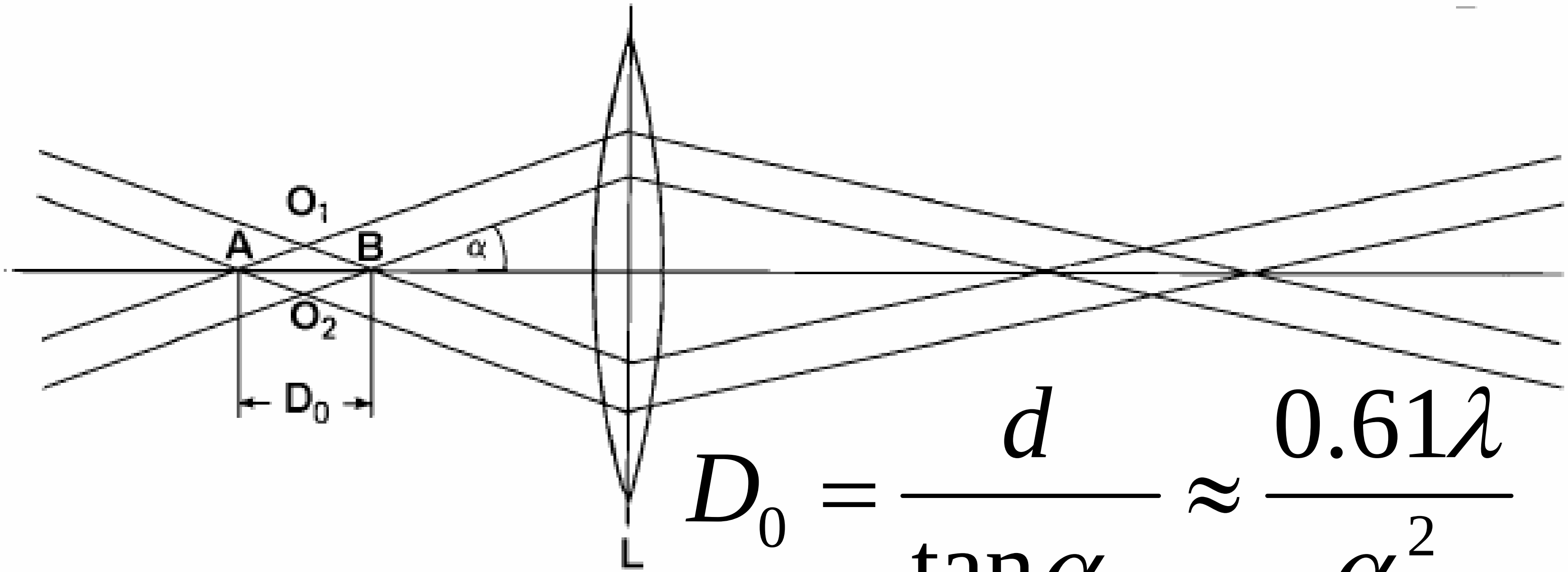


3.11: The normalized rms radius $r_{rms}(C_s\lambda^3)^{-1/4}$ of the STEM probe as a function of the normalized objective aperture $k_{max}(C_s\lambda^3)^{1/4}$ and the normalized defocus $)^{-1/2}$.

$$\Delta f_{\min} = 0.8(C_S\lambda)^{1/2}$$

$$\alpha_{opt} = 1.22\left(\frac{\lambda}{C_3}\right)^{1/4}$$

Depth of Field, Depth of Focus



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

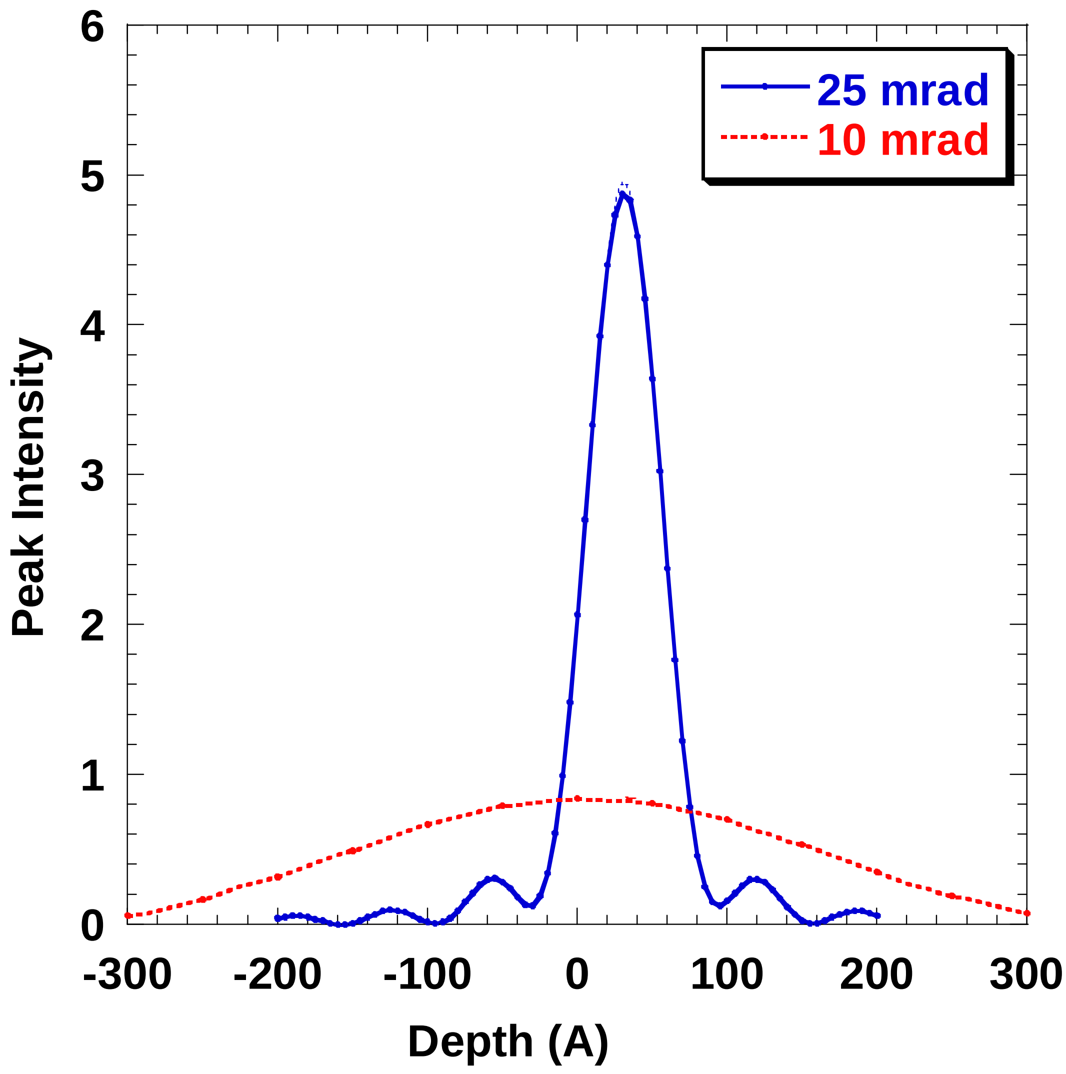
Figure 11. Depth of field. Object points O1 and O2 objects are separated by the resolution limit d of the lens. Rays from these points cross the axis at A and B equally. Hence, points between A and B will look equally sharp, and AB is the depth of field Do of the lens for a semi-angular aperture α.

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!

Depth of Field in ADF-STEM: 3D Microscopy?

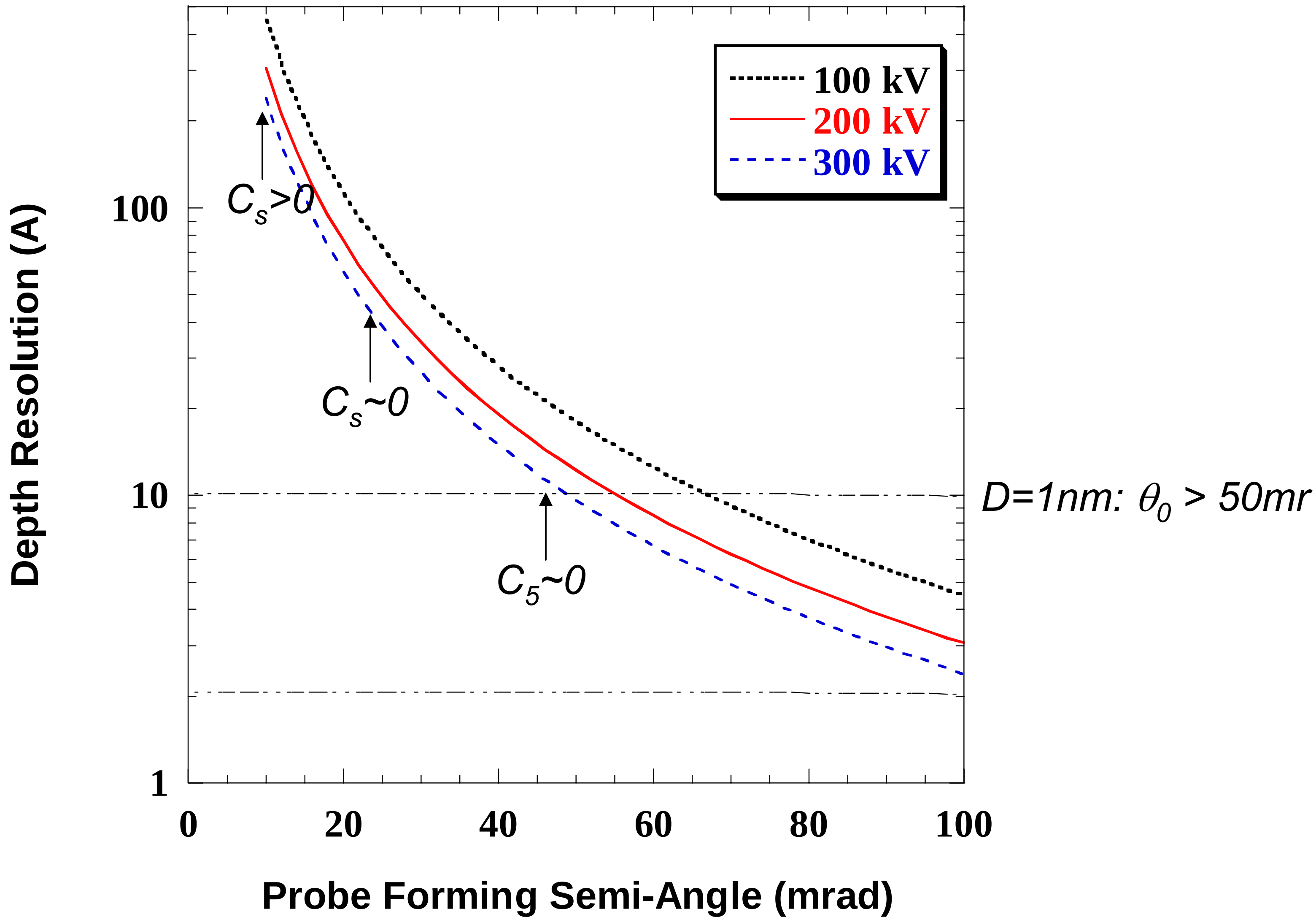
(300 kV, 25 mrad)



D=6 nm: θ_0 *= 25 mr*

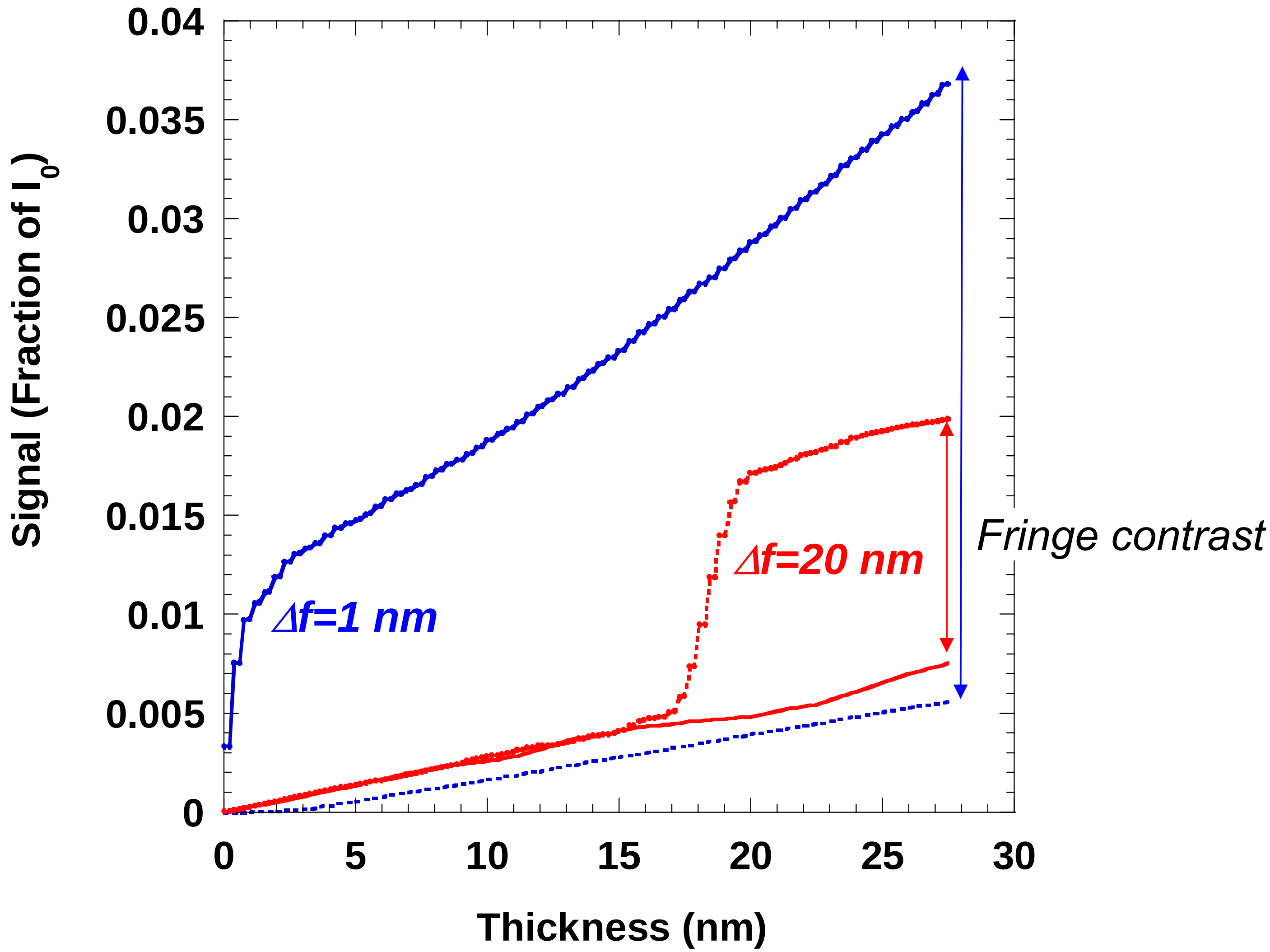
Depth of Field in ADF-STEM: 3D Microscopy?

Today: D~ 6-8 nm   SuperSTEM: ~1 nm



Does Channeling Destroy the 3D Resolution?

(Multislice Simulation of [110] Si @ 200 kV, 50 mrad)



NO! (at least in plane – relative intensities between different depths are still out)

Summary

Contrast Transfer Functions:

Coherent:

$$\alpha_{opt} = \left(\frac{6\lambda}{C_3}\right)^{1/4} \quad d_{\min} = 0.77\, C_3^{1/4} \lambda^{3/4}$$

Lower resolution, higher contrast
Easy to get contrast reversals with defocus
Aperture size only affects cutoff in CTF

Incoherent:

$$\alpha_{opt} = \left(\frac{4\lambda}{C_3}\right)^{1/4} \quad d_{\min} = 0.43\, C_3^{1/4} \lambda^{3/4}$$

Higher resolution, lower contrast
Harder to get contrast reversals with defocus
Aperture size is critical – affects CTF at all frequencies