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

1 atom wide (0.2 nm) beam is scanned across the sample to form a 2-D image

Electron Energy Loss Spectrometer

200 kV Incident Electron Beam ($\Delta E=1$ eV)

Annular Dark Field (ADF) detector

Elastic Scattering $\sim$ "Z contrast"

Increasing energy loss

3 Å


Reciprocity (or STEM vs. CTEM)

Reciprocity (for zero-loss images):
A hollow-cone image in CTEM $\leftrightarrow$ 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:  *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

From L. Reimer, *Transmission Electron Microscopy*
Geometric Optics – A Simple Lens

Focusing: angular deflection of ray $\alpha$ distance from optic axis
Wavefronts in focal plane are the Fourier Transform of the Image/Object
All plane waves at angle $\alpha$ 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)

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

Inverse Transform: (diffraction ->image)

$$f(\vec{x}) = \mathcal{F}^{-1}\{F(\vec{k})\} = \int_{-\infty}^{\infty} F(\vec{k}) e^{-i2\pi \vec{k} \cdot \vec{x}} dS$$

Note: in optics, we define $k=1/d$, while in physics $k=2\pi/d$.
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, $\alpha_{\text{max}}$, and so there is a cut-off spatial frequency $k_{\text{max}} = k_0 \alpha_{\text{max}}$.

$$A(\vec{k}) = \begin{cases} 1, & |\vec{k}| < k_{\text{max}} \\ 0, & |\vec{k}| > k_{\text{max}} \end{cases}$$

$$A(r) = \pi \frac{2J_1(2\pi k_{\text{max}} r)}{2\pi k_{\text{max}} r}$$
The Aperture Function in the Image Plane

\[ A(r) = \pi \frac{2J_1(2\pi k_{\text{max}} r)}{2\pi k_{\text{max}} r} \]

First zero at \( 2\pi k_{\text{max}} r = 0.61 \)

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

David Muller 2006
**Linear Imaging**  (Kirkland chapter 3)

\[ f(x) \rightarrow h(x) \rightarrow g(x) \]

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

- A high-pass filter: Edge-enhancing
  - (multiplication by k in Fourier Space -> differentiation in real space)

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High-pass filter

Original image

Fourier Transform

A high-pass filter

Inverse Transform

Final image

Edge-enhancing
Low pass filter

Original image

Fourier Transform

A low-pass filter

Inverse Transform

Final image

smoothing
The Aperture Function in the Image Plane

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

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

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

i.e. $r = 0.61/(2\pi k_{\text{max}}) \sim 0.61 \lambda/\theta_{\text{max}}$
Adding a central beam-stop to the aperture increases the tails on the probe but only slightly 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 $\beta_{\text{max}}$ (Born&Wolf):

$$\Delta x_{\text{coh}} \approx \frac{0.16 \lambda}{\beta_{\text{max}}}$$

Image resolution

$$d \approx \frac{\lambda}{\alpha_{\text{max}}}$$

Combining these 2 formula we get:

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

Wave Interference inside $\Delta x_{\text{coh}}$ 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:** $\beta_{\text{max}} >> 0.16 \alpha_{\text{max}}$ (usually $\beta_{\text{max}} > 3 \alpha_{\text{max}}$)

No interference, phase shifts are not detected. Intensities add

$$|\psi_a|^2 + |\psi_b|^2$$

David Muller 2006
Coherent Imaging

(Kirkland 3.1)

Lens has a PSF $A(x)$

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

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

We measure the intensity, not the wavefunction

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

Convolve wavefunctions, measure intensities
Incoherent Imaging  
(Kirkland 3.4)

Lost phase information, only work with intensities

\[ \psi_{\text{object}}(x) \]

\[ \psi_{\text{image}}(k) \]

\[ |\psi_{\text{image}}(x)|^2 = |\psi_{\text{object}}(x)|^2 \otimes |A(x)|^2 \]

\[ \psi_{\text{image}}(k) = [\psi_{\text{object}}(k) \otimes \psi_{\text{object}}^*(k)] \cdot [A(k) \otimes A^*(k)] \]

\[ g(x) = \left| \psi_{\text{image}}(x) \right|^2 \]

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

Lens has a PSF \[ |A(x)|^2 \]

We measure the intensity, not the wavefunction

Convolve intensities, measure intensities
## Coherent vs Incoherent Imaging

<table>
<thead>
<tr>
<th></th>
<th>Coherent</th>
<th>Incoherent</th>
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</thead>
<tbody>
<tr>
<td><strong>Point Spread Function</strong></td>
<td>$A(x)$</td>
<td>$</td>
</tr>
<tr>
<td><strong>Contrast Transfer Function</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Phase Object</td>
<td>$\text{Im}[A(k)]$</td>
<td>$</td>
</tr>
<tr>
<td>Amplitude Object</td>
<td>$\text{Re}[A(k)]$</td>
<td></td>
</tr>
<tr>
<td><em>We measure</em></td>
<td>$g(x) =</td>
<td>\psi_{\text{object}}(x) \otimes A(x)</td>
</tr>
</tbody>
</table>
Convolutions
(from Linear Imaging Notes, Braun)

The moving average is obtained by placing the window \( g(x) = (1/a)\text{rect}(x/a) \) 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: \( h(x) = \text{rect}(x) \ast \text{rect}(x) \). 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 $\alpha_0$ is an Airy disk of diameter

$$d_0 = \frac{0.61\lambda}{n \sin \alpha_0} \approx \frac{0.61\lambda}{\alpha_0}$$

(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

<table>
<thead>
<tr>
<th>Accelerating Voltage</th>
<th>v/c</th>
<th>(\lambda) (\text{Å})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 V</td>
<td>0.0019784</td>
<td>12.264</td>
</tr>
<tr>
<td>100 V</td>
<td>0.0062560</td>
<td>1.2263</td>
</tr>
<tr>
<td>1 keV</td>
<td>0.062469</td>
<td>0.38763</td>
</tr>
<tr>
<td>10 keV</td>
<td>0.019194</td>
<td>0.12204</td>
</tr>
<tr>
<td>100 keV</td>
<td>0.54822</td>
<td>0.037013</td>
</tr>
<tr>
<td>200 keV</td>
<td>0.69531</td>
<td>0.025078</td>
</tr>
<tr>
<td>300 keV</td>
<td>0.77653</td>
<td>0.019687</td>
</tr>
<tr>
<td>1 MeV</td>
<td>0.81352</td>
<td>0.0087189</td>
</tr>
</tbody>
</table>
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 $\alpha$, the minimum blur is

$$d_{\text{min}} = \frac{1}{2} C_3 \alpha^3$$

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

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

![Graph showing probe size vs. alpha (mrad)]

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 C₃)

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

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

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

At 200 kV, λ=0.0257 Å, \( d_{\text{min}} = 1.53\text{Å} \) and \( \alpha_{\text{opt}} = 10 \) mrad

At 1 kV, λ=0.38 Å, \( d_{\text{min}} = 12 \text{Å} \) and \( \alpha_{\text{opt}} = 20 \) 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 $\exp[i(2\pi/\lambda)x]$ has a $2\pi$ phase change every $\lambda$)

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)

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

Zernike Polynomials

<table>
<thead>
<tr>
<th>TABLE IV</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Aberrations Corresponding to the First Nine Zernike Terms</strong></td>
</tr>
<tr>
<td>( Z_0 )</td>
</tr>
<tr>
<td>( Z_1 )</td>
</tr>
<tr>
<td>( Z_2 )</td>
</tr>
<tr>
<td>( Z_3 )</td>
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<tr>
<td>( Z_4 )</td>
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<tr>
<td>( Z_5 )</td>
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<tr>
<td>( Z_6 )</td>
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<tr>
<td>( Z_7 )</td>
</tr>
<tr>
<td>( Z_8 )</td>
</tr>
</tbody>
</table>
An Arbitrary Distortion to the Wavefront can be expanded in a power series

Seidel Aberration Coefficients (Seidel 1856)

EM community notation is similar:

\[
\chi(\theta_x, \theta_y) = C_{1,2a}\theta_x\theta_y + C_{2,1a}\frac{\theta_x(\theta_x^2 + \theta_y^2)}{3} + C_{2,1b}\frac{\theta_y(\theta_x^2 + \theta_y^2)}{3} + C_{2,3a}\frac{\theta_x(\theta_x^2 - 3\theta_y^2)}{3} + C_{2,3b}\frac{\theta_y(3\theta_x^2 - \theta_y^2)}{3} + C_3\frac{(\theta_x^2 + \theta_y^2)^2}{4} + C_{3,2a}\frac{\theta_x(\theta_x^4 - \theta_y^4)}{4} + C_{3,2b}\frac{\theta_y(\theta_x^2 + \theta_y^2)^2}{2} + C_{3,4a}\frac{\theta_x^2 \theta_y^2 + \theta_y^2}{4} + C_{3,4b}\frac{\theta_x^3 \theta_y - \theta_x \theta_y^3}{3},
\]

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

Or more generally

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

\( C_{5,0} \) 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

\[ A(\vec{k}) = \begin{cases} e^{i\chi(\vec{k})}, & |\vec{k}| < k_{\text{max}} \\ 0, & |\vec{k}| > k_{\text{max}} \end{cases} \]
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 $\phi/4=\pi/2$, in light optics $\phi/10$

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: \( \Delta f_{opt} = \left( 0.5C_s \lambda \right)^{1/2} \)

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

Minimum Spot size: \( d_{\text{min}} \approx \frac{1.22\lambda}{\alpha_{opt}} \)

\( d_{\text{min}} = 0.77 C_3^{1/4} \lambda^{3/4} \)

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

Optimizing Aperture size with a $C_3$ Corrector

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

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

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

Coherent Imaging CTF: \[ \text{Im}\left[A(k)\right] = \sin[\chi(k)] \]
**Contrast Transfer Functions of a lens with Aberrations**

*Generated with stemtf*

Aperture function of a real lens

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

**Incoherent Imaging CTF:**

\[
\left| A(\vec{k}) \otimes A^*(\vec{k}) \right|^2
\]

---

**CTF for different defocii**

Theorem:

*Aberrations will never Increase the MTF For incoherent imaging*
Phase vs. ADF Contrast

(JEOL 2010F, $C_s=1\text{mm}$)

TEM: Bandpass filter: low frequencies removed = artificial sharpening

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

David Muller 2006
Phase vs. ADF Contrast

Random white noise

BF CTF

ADF CTF

a-C support films look like this
Phase vs. ADF Contrast

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

ADF: 40% narrower FWHM, smaller probe tails
Effect of defocus and aperture size on an ADF-STEM image

(200 kV, \( C_3 = 1.2 \text{ mm} \))

CTF

PSF
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 C₃=1mm)

30% increase in aperture size $\rightarrow$ ~50% decrease in contrast for Si {111} fringes
Aperture Size is Critical
(200 kV C₃=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)

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

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

3.11: The normalized rms radius \( r_{\text{rms}}(C_S \lambda^3)^{-1/4} \) of the STEM probe as a function of the normalized objective aperture \( k_{\text{max}}(C_S \lambda^3)^{1/4} \) and the normalized defocus \( z_{\text{def}}(C_S \lambda^3)^{-1/2} \).
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 \( D_0 \) of the lens for a semi-angular aperture \( \alpha \).

For \( d = 0.2 \) nm, \( \alpha = 10 \) mrad, \( D_0 = 20 \) nm

For \( d = 2 \) nm, \( \alpha = 1 \) mrad, \( D_0 = 2000 \) nm!

For \( d = 0.05 \) nm, \( \alpha = 50 \) mrad, \( D_0 = 1 \) nm!
Depth of Field in ADF-STEM: 3D Microscopy?

(300 kV, 25 mrad)

$D=6 \text{ nm}: \theta_0 = 25 \text{ mrad}$
Depth of Field in ADF-STEM: 3D Microscopy?

Today: $D \sim 6-8 \text{ nm}$        SuperSTEM: $\sim 1 \text{ nm}$

$\theta_0 > 50 \text{ mrad}$

$C_s \sim 0$

$C_5 \sim 0$

$D = 1 \text{ nm}$: $C_0 > 50 \text{ mrad}$

Depth of Field vs. Probe Forming Semi-Angle (mrad)

$100 \text{ kV}$

$200 \text{ kV}$

$300 \text{ kV}$
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:

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

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

Incoherent:

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

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