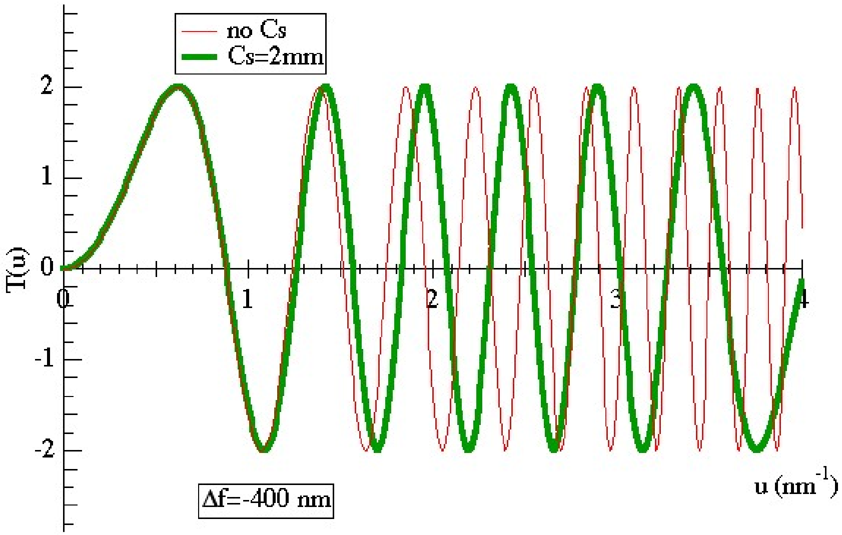
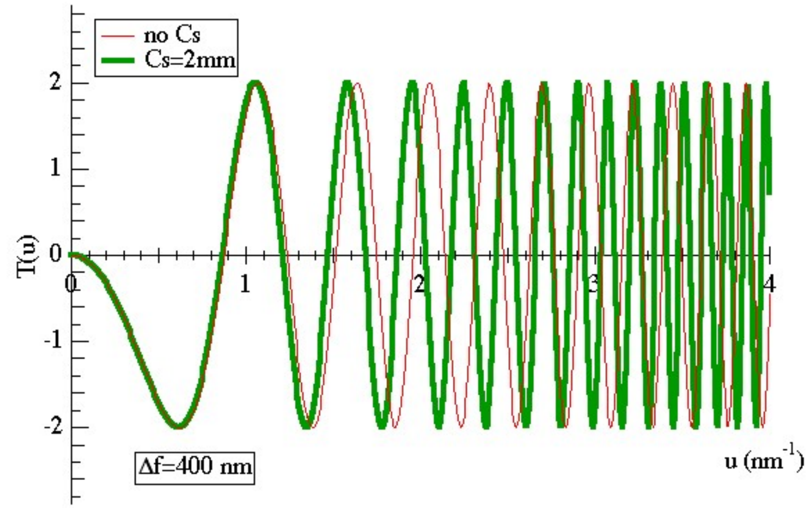
Influence of C_s

$\Delta f < 0$



$\Delta f > 0$



oscillations are faster in overfocus

$$T(u,\Delta f) \approx -2\sin\left[\chi(u,\Delta f)\right]$$

$$\chi(u,\Delta f) = \pi \cdot \left(\Delta f \cdot \lambda \cdot u^2 + \frac{1}{2} C_s \cdot \lambda^3 \cdot u^4\right)$$

Finding C_s, Δf

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

$$T(u) = -2\sin\left[\chi(u)\right]$$

Maxima: $\sin\chi(u) = \pm 1 \Rightarrow \chi(u) = \left(n + \frac{1}{2}\right)\cdot\pi$

Zeros: $\sin\chi(u) = 0 \Rightarrow \chi(u) = n\pi$ $\quad n \in \mathbb{Z}$

The zeros should occur at frequencies where:

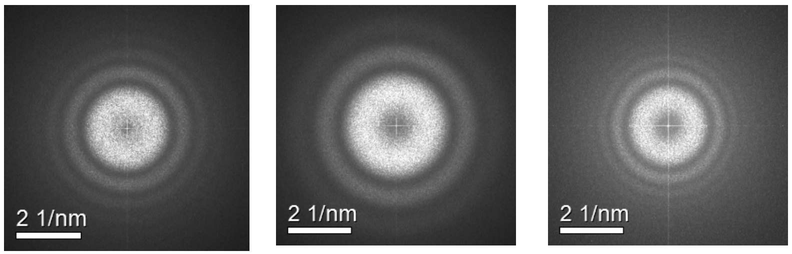
$$n = \Delta f \cdot \lambda \cdot \left(u^2\right) + \frac{1}{2} C_s \cdot \lambda^3 \cdot \left(u^2\right)^2$$

Measure C_s: JEM-2100

FFTs of images from a-C films

underfocus ← | → *overfocus*

Δf=-196 nm Δf=-130 nm Δf=207 nm



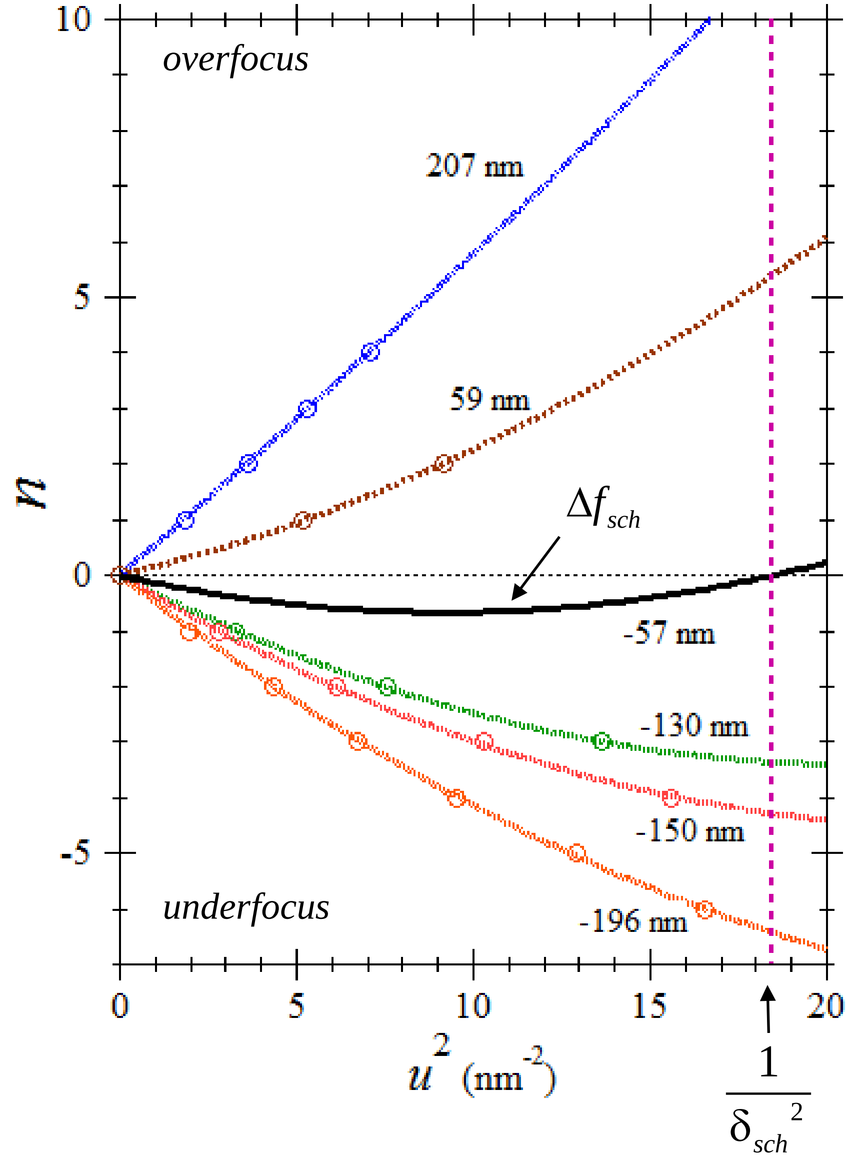
Fit: $$n = \Delta f \cdot \lambda \cdot (u^2) + \frac{1}{2} C_s \cdot \lambda^3 \cdot (u^2)^2$$

$$E = 200 \text{ KeV}$$

$$C_s = 0.99 \text{ mm}$$

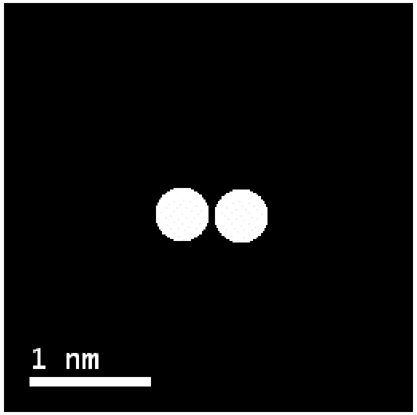
$$\Delta f_{sch} = -\left(\frac{4}{3} C_s \lambda\right)^{1/2} = -57 \text{ nm}$$

$$\delta_{sch} = 0.66\left(C_s \lambda^3\right)^{1/4} = 0.23 \text{ nm}$$



Example: Phase Contrast

$V(x,y)$



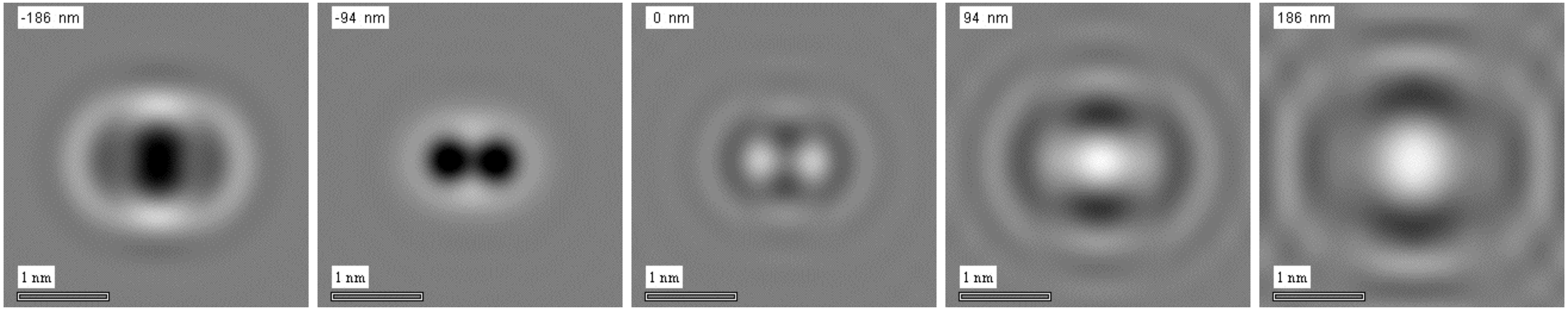
$E = 125$ KeV

$C_s = 2.0$ mm

$\Delta f_{sch} = -93.7$ nm

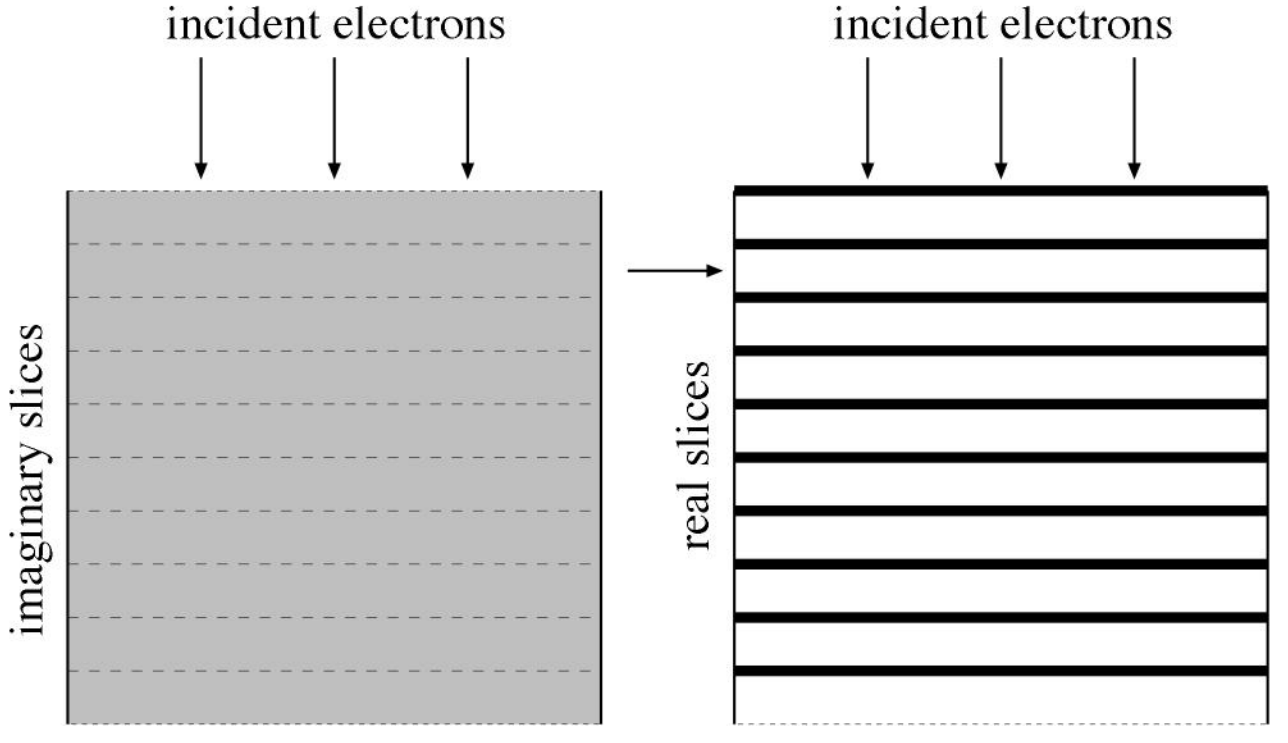
$\delta_{sch} = 0.34$ nm

$\Delta f = -2|\Delta f_{sch}|$ $\Delta f = -|\Delta f_{sch}|$ $\Delta f = 0$ $\Delta f = |\Delta f_{sch}|$ $\Delta f = |2\Delta f_{sch}|$



Multislice Method

•Consider specimen to contain many thin slices
•Project potential onto a plane above each slice
•Propagate the wave through the vacuum between slices



Multislice Propagation

slice

1 $\psi_0(x,y)$

$f_1(x,y)\psi_0(x,y)$

Δz_1

2 $\psi_1(x,y) = p(x,y,\Delta z_1) * \left[f_1(x,y)\psi_0(x,y) \right]$

$f_2(x,y)\psi_1(x,y)$

Δz_2

3 $\psi_2(x,y) = p(x,y,\Delta z_2) * \left[f_2(x,y)\psi_1(x,y) \right]$

$f_3(x,y)\psi_2(x,y)$

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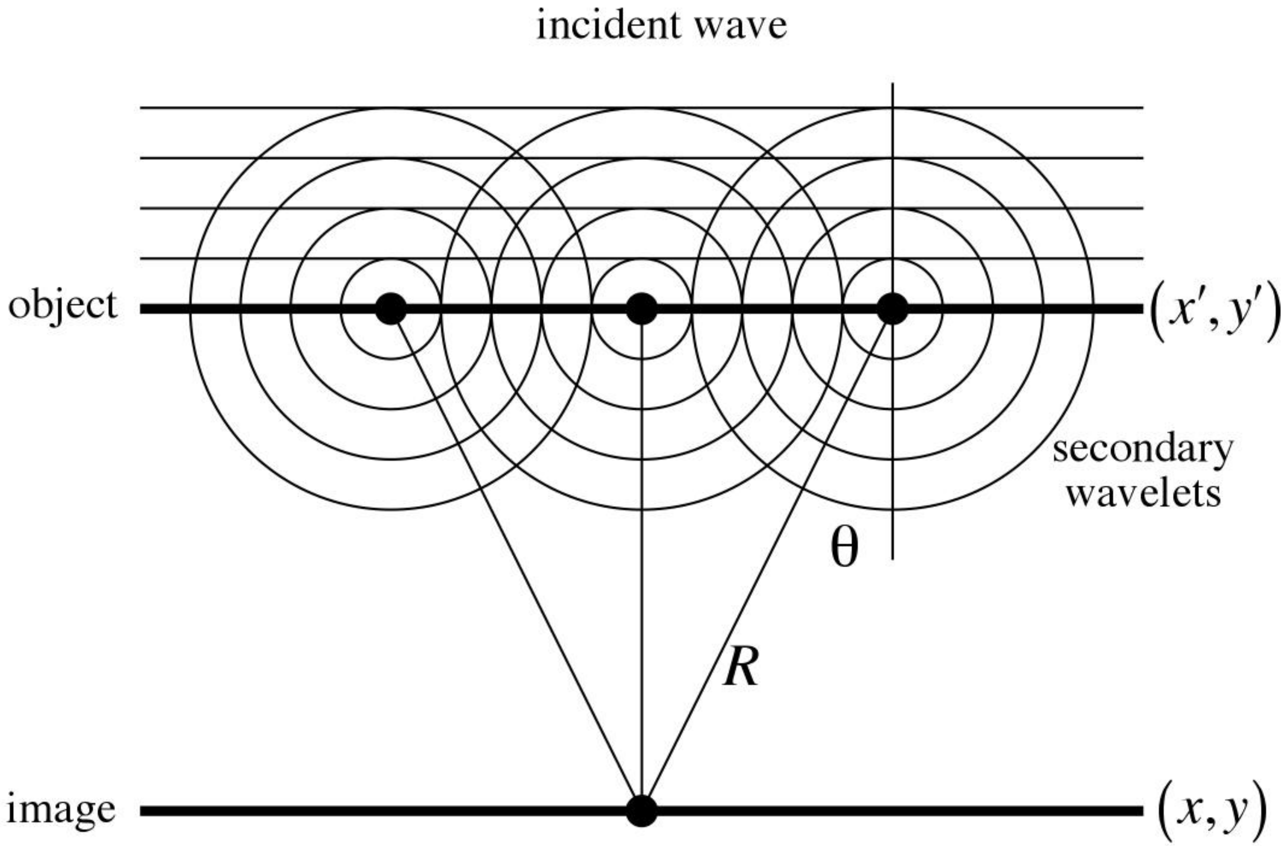
Propagator

Huygens' Principle: Each point on the wave front acts as a source of secondary, spherical wavelets



Deriving the propagator

Fresnel-Kirchhoff integral: $$\psi(x,y,z+\Delta z) = -ik \int_{source} \psi(x',y',z) \cdot \frac{e^{2\pi ikR}}{R} \cdot \left(\frac{1+\cos\theta}{2}\right) dx'dy'$$

Small-angle approximation: $$R = \sqrt{(x-x')^2 + (y-y')^2 + (\Delta z)^2}$$

obliquity factor: $\frac{1+\cos\theta}{2} \approx 1$

$$e^{2\pi ikR} \approx e^{2\pi ik\cdot\Delta z} \cdot e^{\pi ik\cdot\Delta z\cdot\left[\left(\frac{x-x'}{\Delta z}\right)^2 + \left(\frac{y-y'}{\Delta z}\right)^2\right]}$$

$$\frac{1}{R} \approx \frac{1}{\Delta z} \cdot \left[1 - \frac{1}{2}\left(\frac{x-x'}{\Delta z}\right)^2 - \frac{1}{2}\left(\frac{y-y'}{\Delta z}\right)^2\right]$$

$$\frac{e^{2\pi ikR}}{R} \approx \frac{e^{2\pi ik\cdot\Delta z} \cdot e^{\frac{\pi ik}{\Delta z}\left[(x-x')^2 + (y-y')^2\right]}}{\Delta z}$$

$$\psi(x,y,z+\Delta z) \approx -ik \frac{e^{2\pi ik\cdot\Delta z}}{\Delta z} \int_{x',y'} \psi(x',y',z) \cdot e^{\frac{\pi ik}{\Delta z}\left[(x-x')^2 + (y-y')^2\right]} dx'dy'$$

This is a convolution.

The Propagator Function

The convolution can be written as:

$$\psi(x, y, z+\Delta z) = e^{2\pi i k \cdot \Delta z} \int_{x', y'} \psi(x', y', z) \cdot p(x - x', y - y') \, dx' dy'$$

$$p(x, y) \equiv \frac{-ik}{\Delta z} \cdot e^{\frac{\pi i k}{\Delta z}\left(x^2 + y^2\right)}$$

We drop the phase factor: $e^{2\pi i k \cdot \Delta z}$

$$\psi(x, y, z+\Delta z) = \psi(x, y, z) * p(x, y, \Delta z)$$

Multislice algorithm

$$\psi_{n+1}(x,y) = p(x,y,\Delta z_{n+1}) * \left[f_{n+1}(x,y) \cdot \psi_n(x,y) \right]$$

1) Transmit through projected potential
2) Propagate through vacuum
repeat

$$\psi_1 = p(\Delta z_1) * [f_1 \cdot \psi_0]$$

$$\psi_2 = p(\Delta z_2) * [f_2 \cdot \psi_1] = p(\Delta z_2) * \left[f_2 \cdot \left[p(\Delta z_1) * [f_1 \cdot \psi_0] \right] \right]$$

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Multislice in reciprocal space

The FT of a convolution is the product of the FTs

$$\Im\left\{\psi_{n+1}(x,y)\right\} = \Im\left\{p(x,y,\Delta z)\right\} \cdot \Im\left\{f_{n+1}(x,y) \cdot \psi_n(x,y)\right\}$$

FT of propagator: $\Im\left\{p(x,y,\Delta z)\right\} = p\left(u_x, u_y, \Delta z\right) = \mathrm{e}^{-\pi i\left(u_x{}^2 + u_y{}^2\right)\Delta z / k}$

$$\psi_{n+1}(x,y) = \Im^{-1}\left\{\mathrm{e}^{-\pi i\left(u_x{}^2 + u_y{}^2\right)\Delta z_n / k} \cdot \Im\left\{f_{n+1}(x,y) \cdot \psi_n(x,y)\right\}\right\}$$

Multiply, transform, multiply, inverse transform

Periodic boundary conditions needed to use FFT without artifacts.

Some atoms (e.g., Au) may not be not pure phase objects

Simulations: spherical particle, multislice

$E = 200$ KeV

$C_s = 2.0$ mm

$\Delta f_{sch} = -82$ nm

$\alpha_{damp} = 2.0\ \text{nm}^{-1}$

$\Delta f = -|\Delta f_{sch}|$ $\Delta f = 0$ $\Delta f = |\Delta f_{sch}|$

$|g|^2$

FFT