More on phase contrast

In vacuum:

$$k = \sqrt{\frac{2mE_{nr}}{h^2}}$$

$$E_{nr} = \left(\frac{m + m_0}{2m}\right) \cdot E$$

In the specimen:

$$K(\mathbf{r}) = \sqrt{\frac{2m\left[E_{nr} + eV(\mathbf{r})\right]}{h^2}}$$

$$= k\sqrt{1 + \frac{eV(\mathbf{r})}{E_{nr}}}$$

$$K(\mathbf{r}) \approx k\left[1 + \frac{eV(\mathbf{r})}{2E_{nr}}\right] = k + \frac{\sigma V(\mathbf{r})}{2\pi}$$

Interaction constant: $\sigma \doteq \dfrac{\pi k e}{E_{nr}}$

The wave number in the specimen is not a constant

Phase object approximation

For an increment *dz* in thickness:

$$\psi\left(x, z+dz\right) = \psi\left(x, z\right)\mathrm{e}^{2\pi i K(\mathbf{r})dz} \approx \psi\left(x, z\right)\mathrm{e}^{2\pi i k\cdot dz}\mathrm{e}^{i\sigma V(\mathbf{r})dz}$$

Find the net phase change by integrating over the entire thickness *T*:

$$\psi\left(x, z+dz\right) \rightarrow \psi + d\psi$$

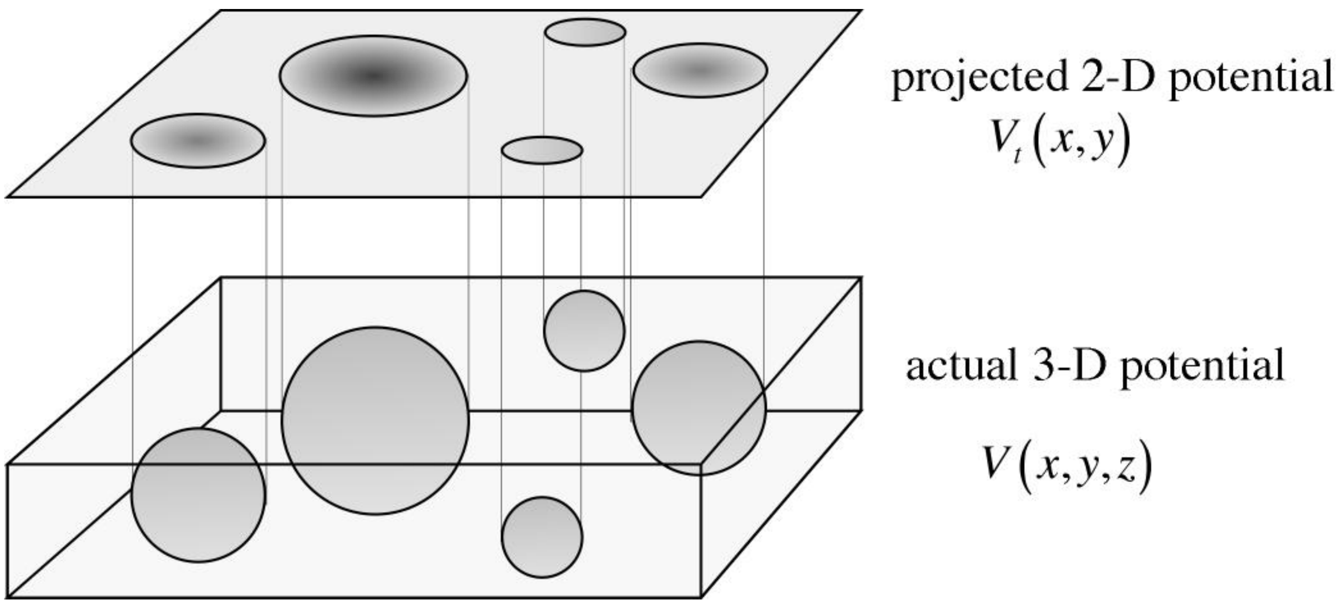
$$\psi + d\psi = \psi \cdot \mathrm{e}^{2\pi i K(\mathbf{r})dz}$$

$$\cancel{\psi} + d\psi \approx \psi \cdot \left[\cancel{1} + 2\pi i K\left(\mathbf{r}\right)dz\right]$$

$$\int_{\psi=\psi(x,0)}^{\psi(x,T)} \frac{d\psi}{\psi} = \int_{z=0}^{T} 2\pi i K\left(\mathbf{r}\right)\cdot dz = \int_{z=0}^{T} 2\pi i\left[k + \frac{\sigma V\left(\mathbf{r}\right)}{2\pi}\right]\cdot dz$$

$$\ln\left[\frac{\psi\left(x,T\right)}{\psi\left(x,0\right)}\right] = 2\pi i k T + i\sigma\int_{z=0}^{T} V\left(\mathbf{r}\right)\cdot dz$$

Projected Potential



$$V_t(x,y) \doteq \int_{z=0}^{T} V(x,y,z) \cdot dz$$

Applying the phase-object approximation

$$\psi(x,T) = \psi(x,0) \cdot \mathrm{e}^{2\pi i k \cdot T} \cdot \mathrm{e}^{i\sigma V_t(x)}$$

Final (exit) wave: $\psi_f = \psi(x,T)$

Initial (unscattered) wave: $\psi_i = \psi(x,0) \cdot \mathrm{e}^{2\pi i k \cdot T}$

Specimen (object) function: $F(x) = \mathrm{e}^{i\sigma V_t(x)}$

$$\psi_f(x) = F(x) \cdot \psi_i$$

WPOA

object function: $F(x) = \mathrm{e}^{i\sigma V_t(x)} \approx 1 + i\sigma V_t(x)$ $\quad \sigma V_t(x) \ll 1$

exit wave:

$$\psi_f(x) \approx \left[1 + i\sigma V_t(x)\right] \cdot \psi_i = \psi_i + i\psi_{sc}(x) \qquad \psi_{sc}(x) \ll \psi_i$$

Normalize: $1 = |\psi_i|^2 + \underbrace{\cancel{|\psi_{sc}(x)|^2}}^{small}$ $\quad \rightarrow \psi_i = 1$

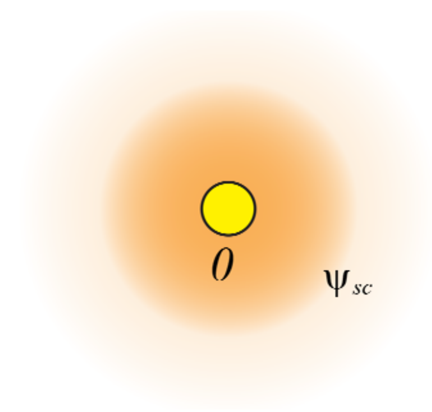
$$\longrightarrow \quad F(x) = \psi_i + i\psi_{sc}(x)$$

image function: $G(x) = \psi_i + i\psi_{sc}(x) \cdot \mathrm{e}^{-i\chi}$

additional phase change
due to objective lens

Phase contrast

$$F(x) = \psi_i + i\psi_{sc}(x)$$



$$G(x) = \psi_i + i\psi_{sc}(x)\cdot e^{-i\chi}$$

$$I(x) = |G(x)|^2$$

$$= \left|1 + i\psi_{sc}(x)\cdot e^{-i\chi}\right|^2 \qquad (\psi_i = 1)$$

$$= 1 + \cancel{|\psi_{sc}(x)|^2} + i\psi_{sc}(x)\cdot e^{-i\chi} - i[\psi_{sc}(x)]^*\cdot e^{i\chi}$$

$$I(x) = 1 - 2\,\mathrm{Im}\left[\psi_{sc}(x)\cdot e^{-i\chi}\right]$$

Assume $\psi_{sc}(x)$ is real:

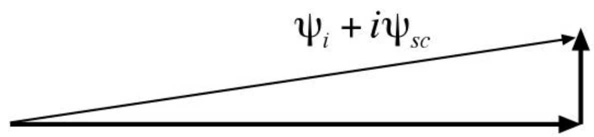
$$I(x) = 1 + 2\psi_{sc}(x)\sin(\chi)$$

Phase contrast

Phase shifts due to focus of objective lens affect contrast:

<u>in focus</u>

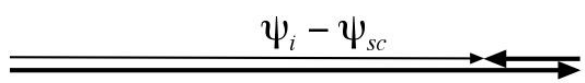
$$\chi = 0$$



No phase contrast

<u>underfocus</u>

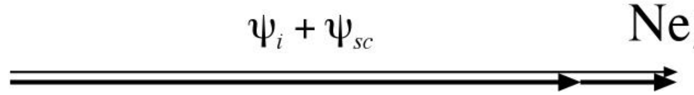
$$\chi = -\pi/2$$



Positive phase contrast

<u>overfocus</u>

$$\chi = \pi/2$$

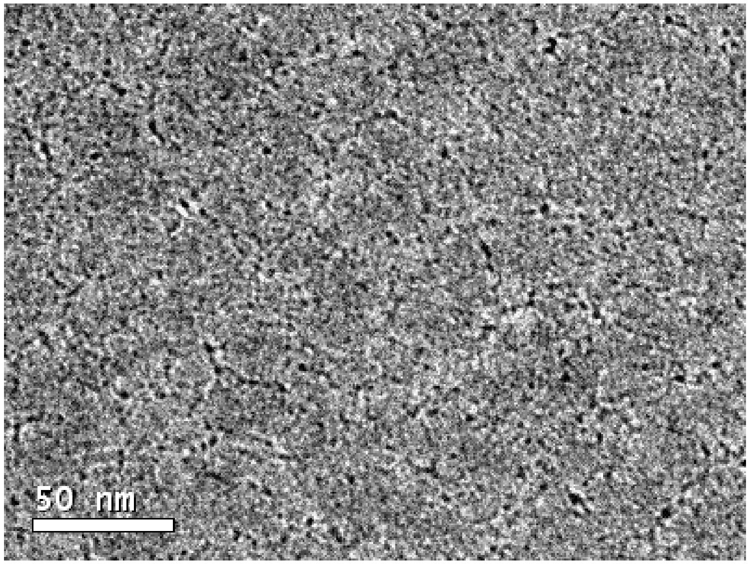


Negative phase contrast

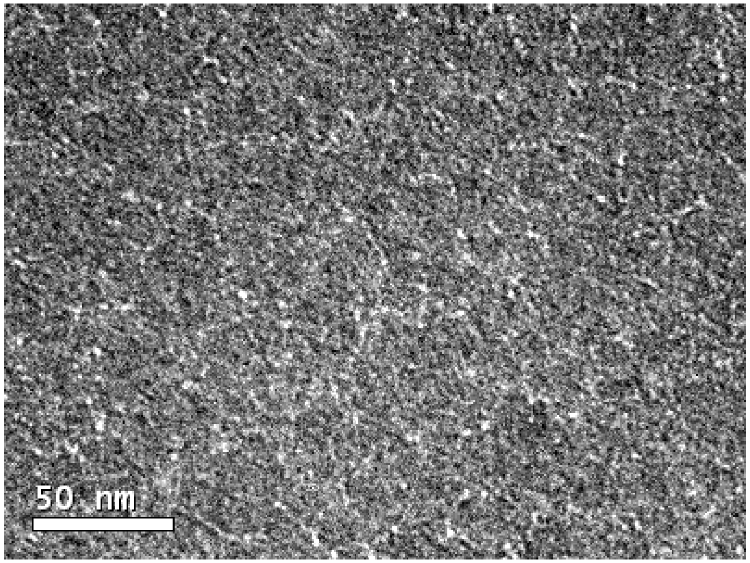
Objective lens provides additional phase shift needed for positive phase contrast

Phase Contrast Example I: a-C

Underfocus-positive phase contrast



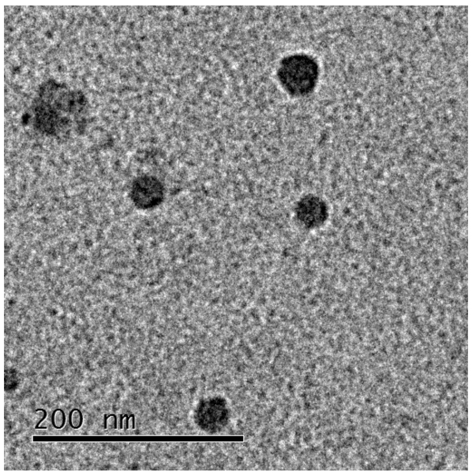
Overfocus-negative phase contrast



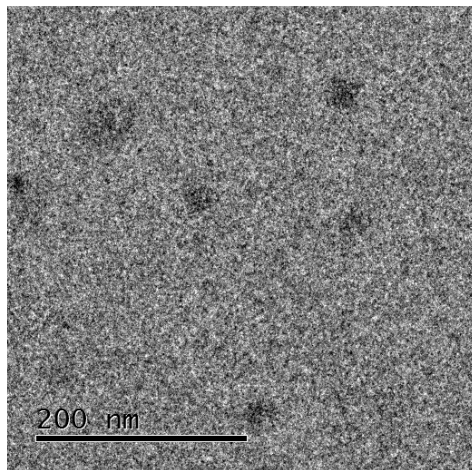
Contrast Reversal

Phase Contrast Example II: polystyrene spheres

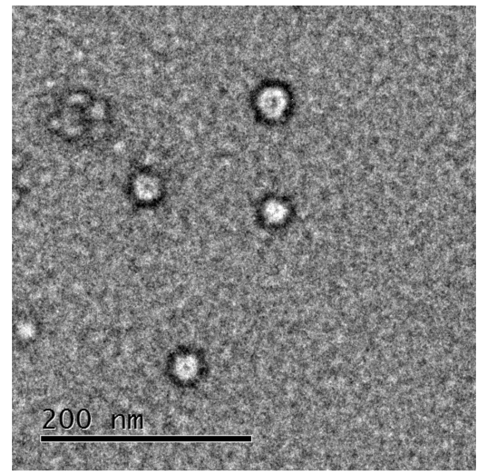
Underfocus



In Focus



Overfocus

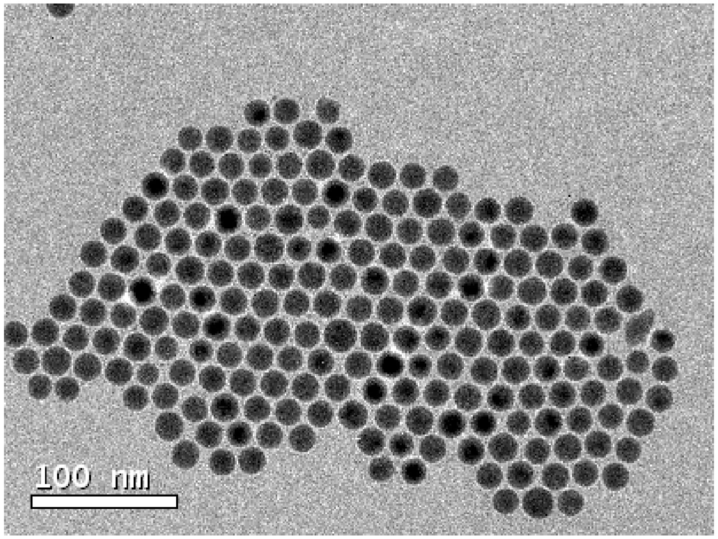


Contrast Reversal

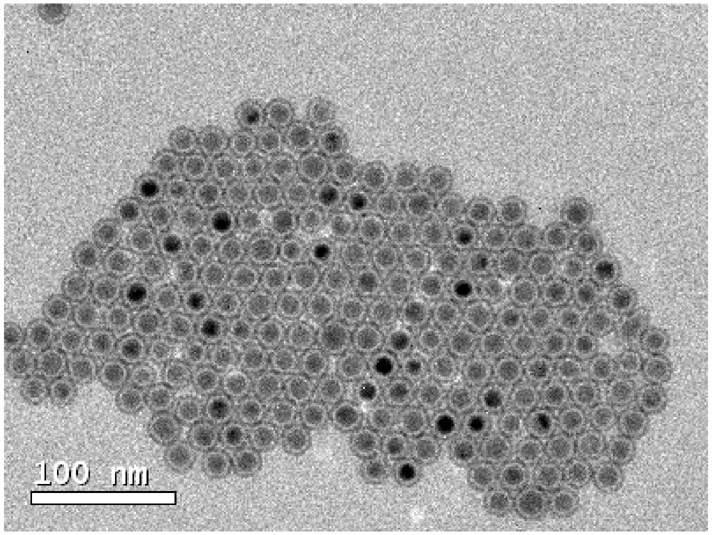
Other differences, such as "Fresnel fringes" at edges, result from spherical aberration.

Not Pure Phase Objects

Slightly underfocus



Overfocus

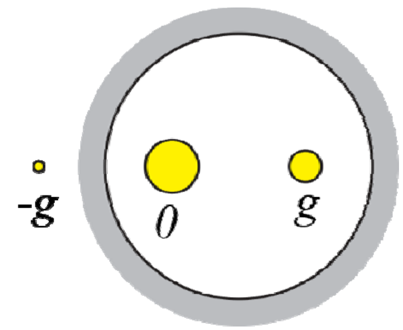


Lattice fringes (two-beam)

Two-beam: $F(x) \approx \left\{\Psi_0(T) + \left[\Psi_g(T)\cdot \mathrm{e}^{2\pi isT}\right]\cdot \mathrm{e}^{2\pi igx}\right\}\cdot \mathrm{e}^{2\pi ikT} \rightarrow 1 + i\phi_g \cdot \mathrm{e}^{2\pi igx}$

$\phi_g = \left|\phi_g\right| \cdot \mathrm{e}^{i\delta}$ $\qquad$ $\psi_{sc}(x) = \phi_g \cdot \mathrm{e}^{2\pi igx} = \left|\phi_g\right| \cdot \mathrm{e}^{i(2\pi gx+\delta)}$ //complex

$$G(x) = 1 + i\left|\phi_g\right| \cdot \mathrm{e}^{i(2\pi gx+\delta-\chi)}$$



$$\begin{aligned} I(x) &= 1 - 2\,\mathrm{Im}\left[\psi_{sc}(x)\cdot \mathrm{e}^{-i\chi}\right] \\ &= 1 - 2\,\mathrm{Im}\left[\left|\phi_g\right| \cdot \mathrm{e}^{i(2\pi gx+\delta-\chi)}\right] \end{aligned}$$

$$I(x) = 1 + 2\left|\phi_g\right| \cdot \sin(2\pi gx + \delta - \chi)$$

(fringes!)

Fringes shift laterally as focus (χ) is changed

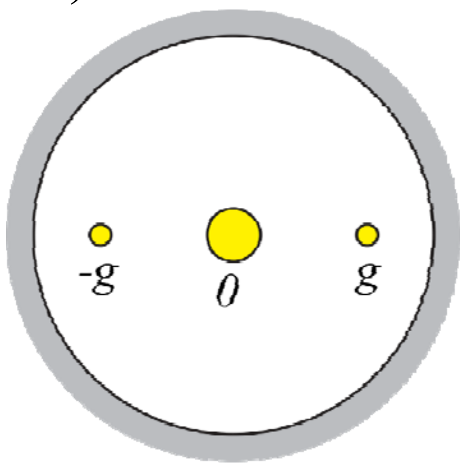
Lattice fringes (three-beam)

Three-beam (*0* and *g and -g*): $F(x) \to 1 + i\phi_g \cdot \mathrm{e}^{2\pi igx} + i\phi_{-g} \cdot \mathrm{e}^{-2\pi igx}$

$$\phi_{-g} = \left|\phi_g\right| \cdot \mathrm{e}^{-i\delta}$$

$$\psi_{sc}(x) = \phi_g \cdot \mathrm{e}^{2\pi igx} + \phi_{-g} \cdot \mathrm{e}^{-2\pi igx} = 2\left|\phi_g\right| \cdot \cos(2\pi gx + \delta)$$

$$I(x) = 1 - 2\,\mathrm{Im}\left[\psi_{sc}(x) \cdot \mathrm{e}^{-i\chi}\right]$$
$$= 1 - 2\,\mathrm{Im}\left[2\left|\phi_g\right| \cdot \cos(2\pi gx + \delta) \cdot \mathrm{e}^{-i\chi}\right]$$
$$I(x) = 1 + 4\left|\phi_g\right| \cdot \cos(2\pi gx + \delta) \cdot \sin(\chi)$$



Fringe contrast: $\begin{cases} \text{positive phase contrast,} & \chi < 0 \\ \text{no contrast,} & \chi = 0 \\ \text{negative phase contrast,} & \chi < 0 \end{cases}$

No lateral shifting of fringes.

HR lattice image example