Simulation of Dynamical Scattering Effect in Electron Diffraction Patterns

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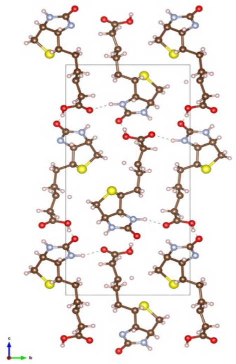
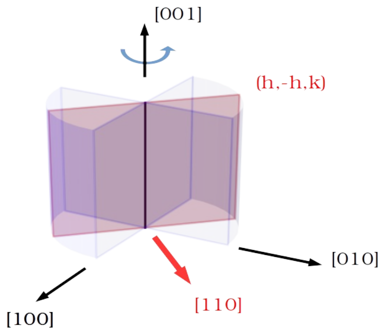
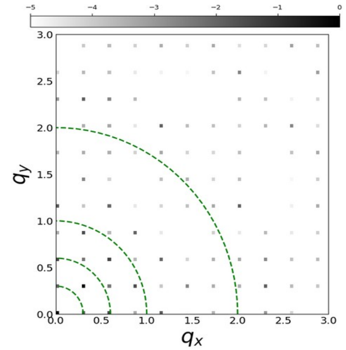


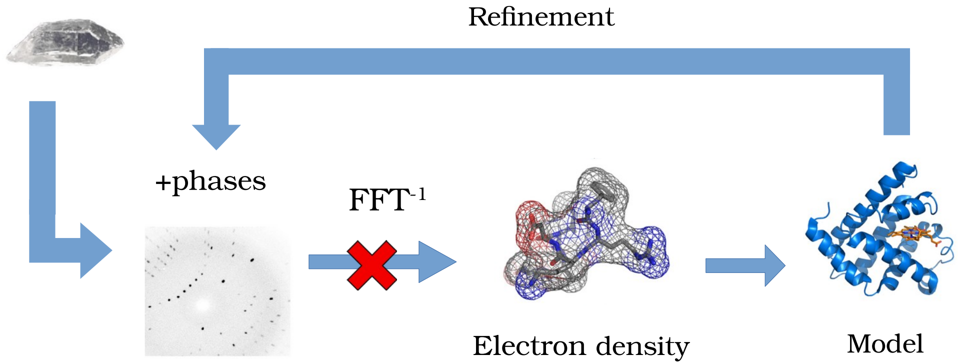




UK Research and Innovation

Numerical simulation tools of ED patterns

Kinematic approximation



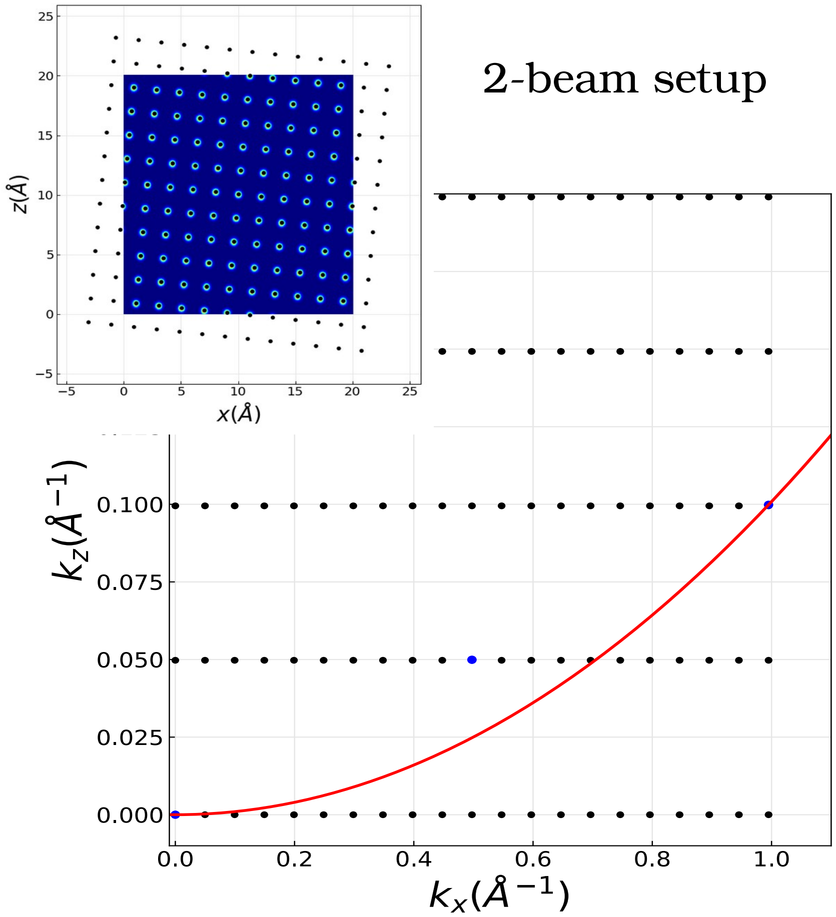
Schrodinger's fast electron wave equation

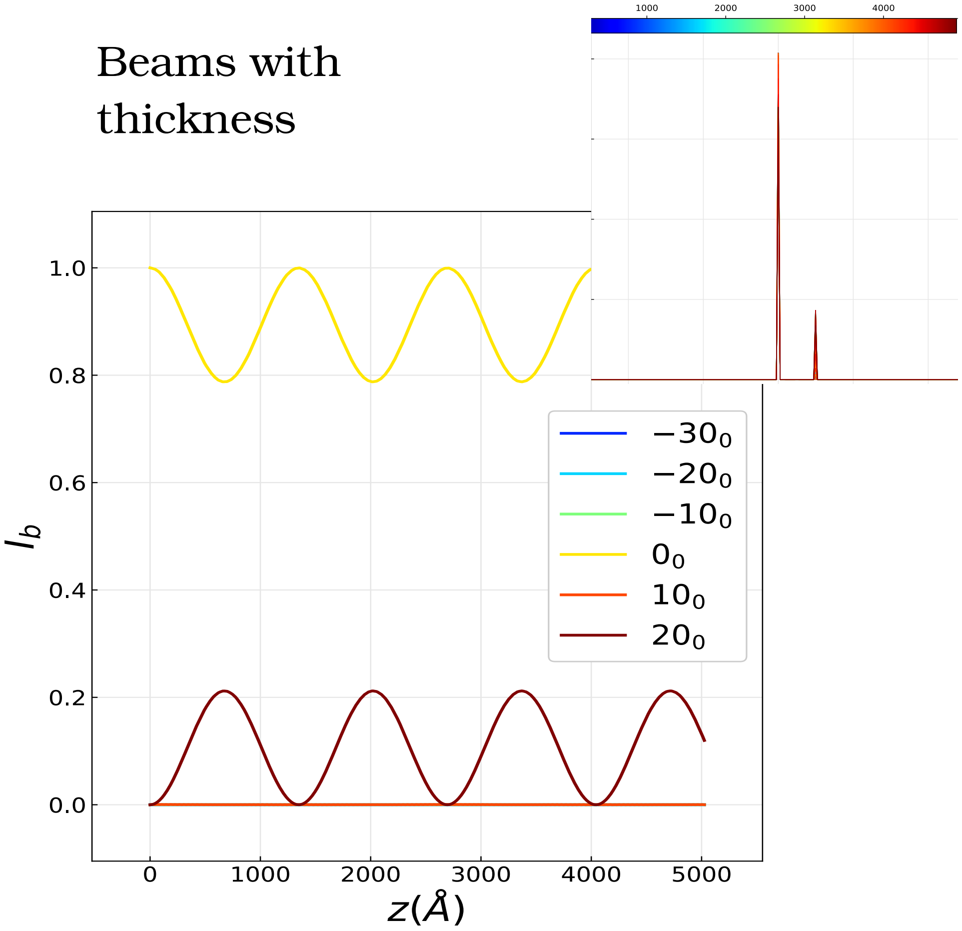
$$\left\{\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r})\right\}\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \quad \xrightarrow[\partial_z^2 \ll 2ik_0\partial_z]{} \quad \frac{\partial\Psi(x,y,z)}{\partial_z} = \left\{\frac{i\lambda}{4\pi}\nabla^2_{xy} + i\sigma V(x,y,z)\right\}\Psi(x,y,z)$$

Numerical simulation tools of ED patterns

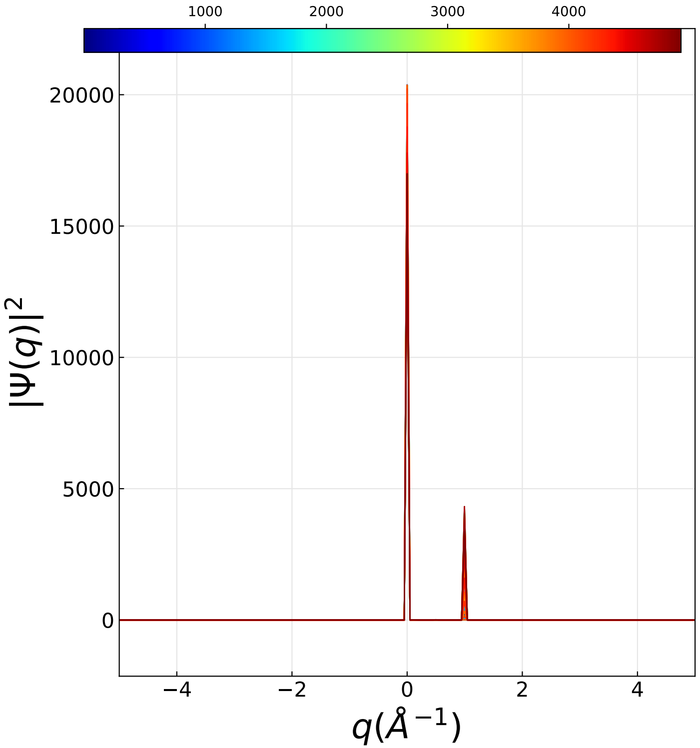
Method	Exact	Speed	Mem (beam per atom)	Periodic structure	Grid based	Parallelization type	Package
Multislice (MS) (physical optics based approach)	no	$N_z N_b \log N_b$	100	**yes**	**yes**	FFTw one slice after another	**TEMSIM (pyMS)** PRISM,...
Near bragg (real space path differences)	no	$N_z N_b^2 N_p$	1	**no**	**no**	per pixel	NearBragg (James Holton)

Multislice 2-beam diffraction case

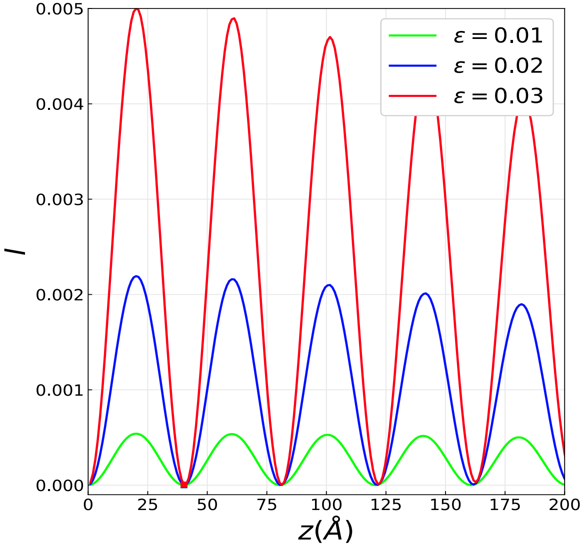




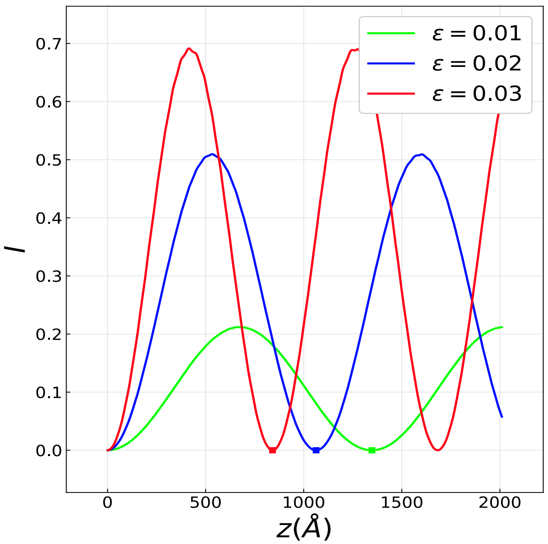
Dynamical diffraction extinction distance



Kinematic Ewald sphere curvature effect weakly diffracted beam



Potential dependent extinction distance for strongly diffracting beam

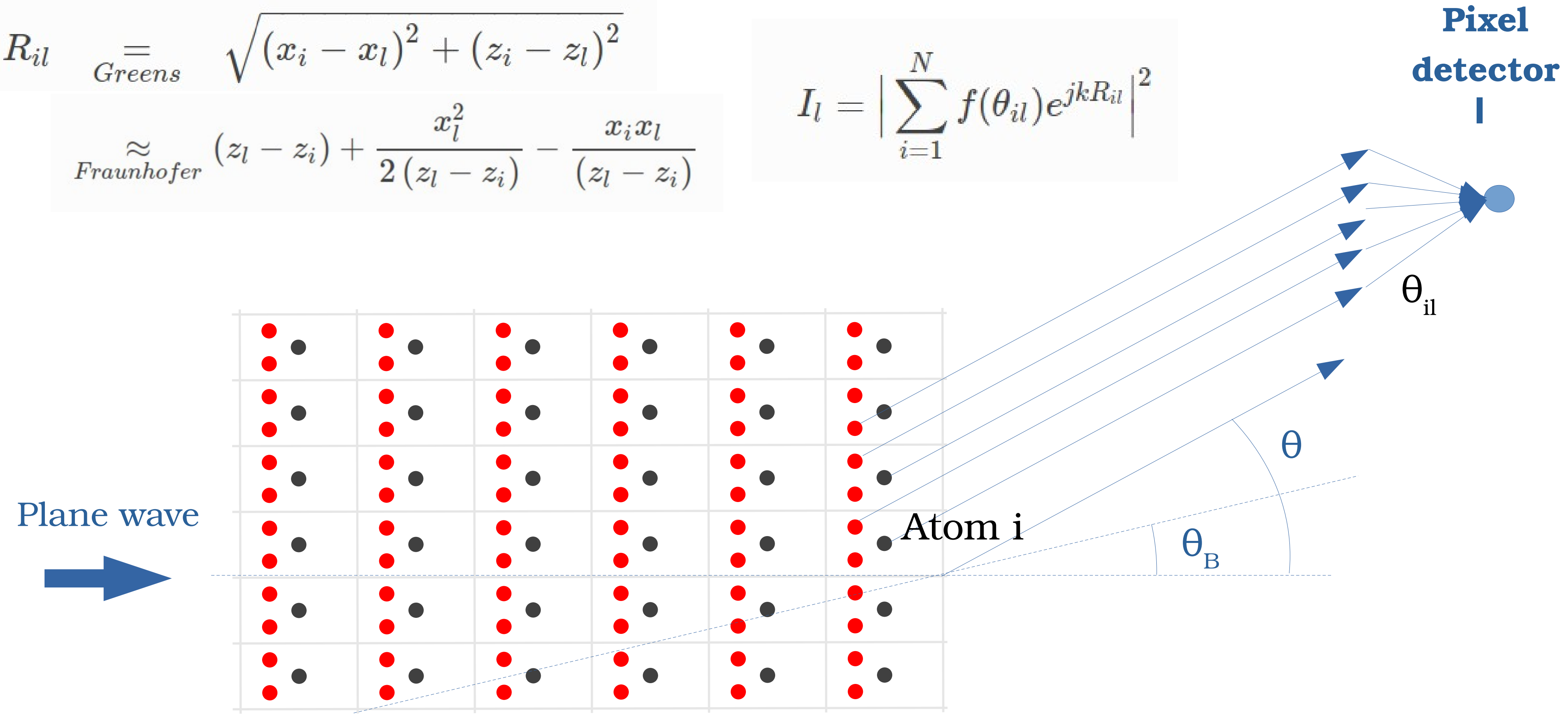


Near Bragg

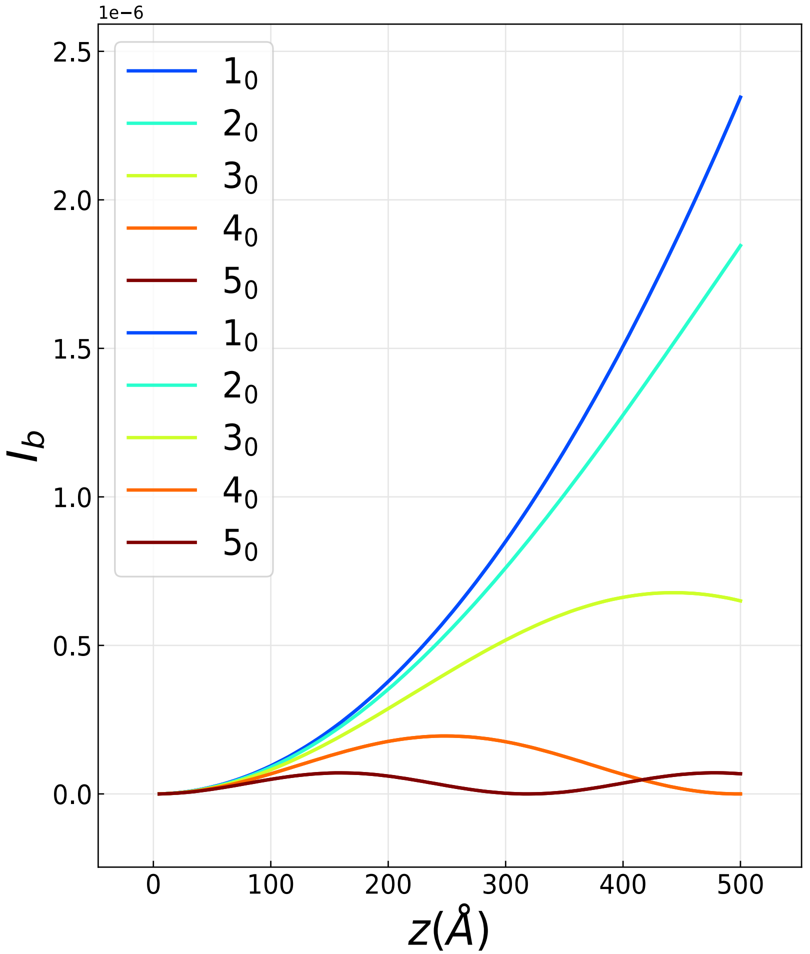
$$R_{il} \underset{Greens}{=} \sqrt{(x_i - x_l)^2 + (z_i - z_l)^2}$$

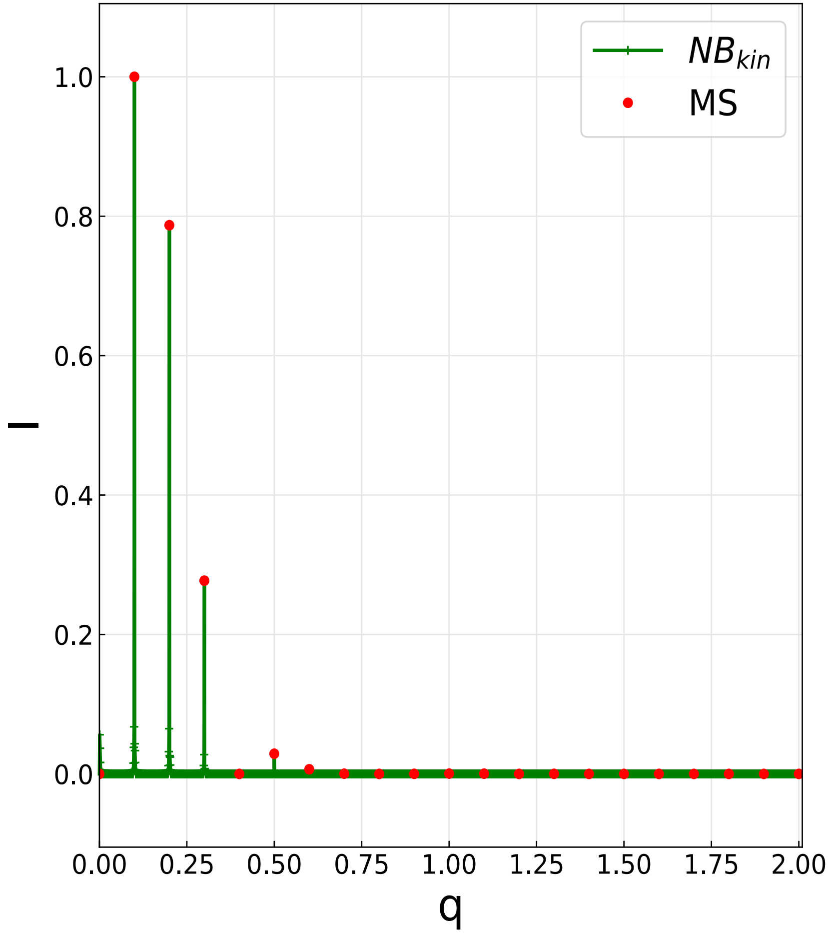
$$\underset{Fraunhofer}{\approx} (z_l - z_i) + \frac{x_l^2}{2\,(z_l - z_i)} - \frac{x_i x_l}{(z_l - z_i)}$$

$$I_l = \left| \sum_{i=1}^{N} f(\theta_{il}) e^{jkR_{il}} \right|^2$$

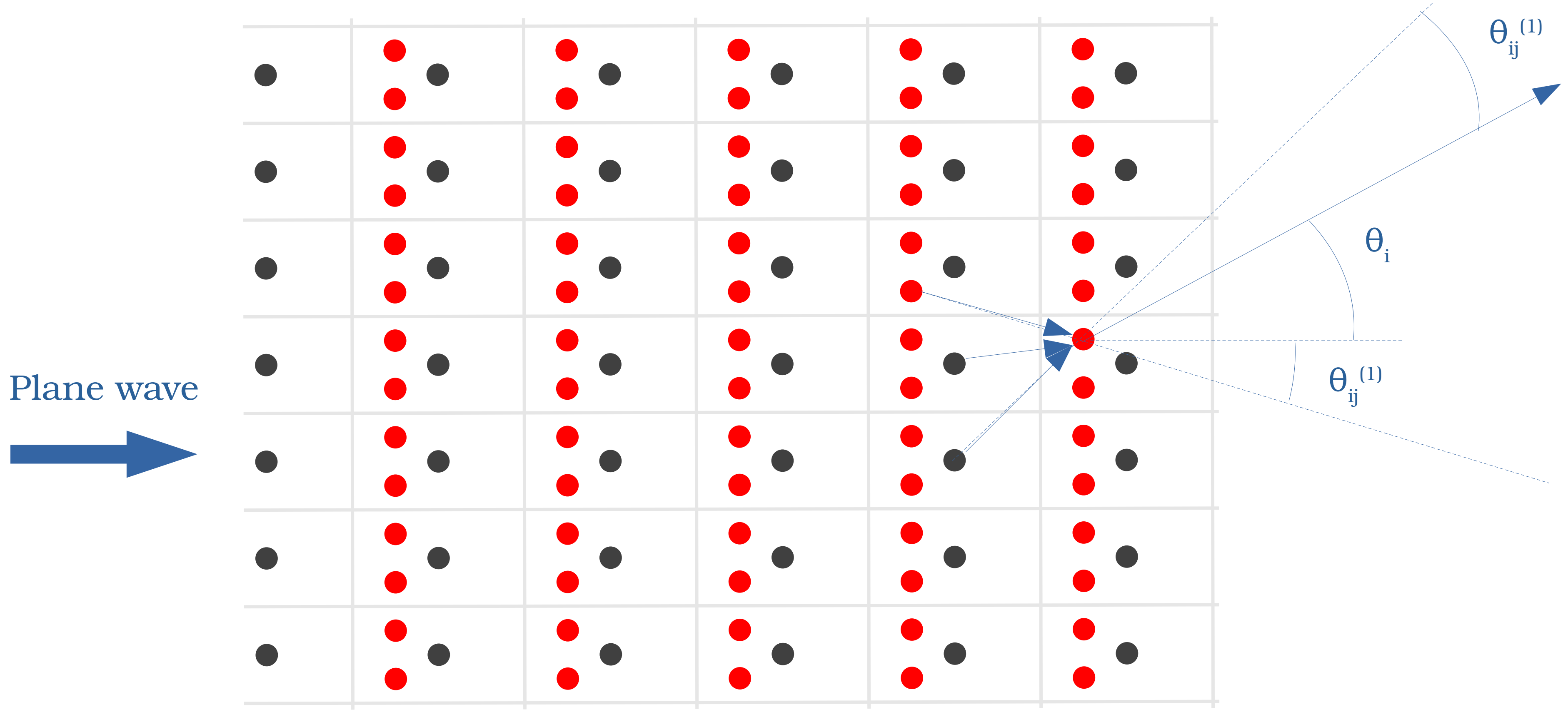


Weak potential kinematic approximation





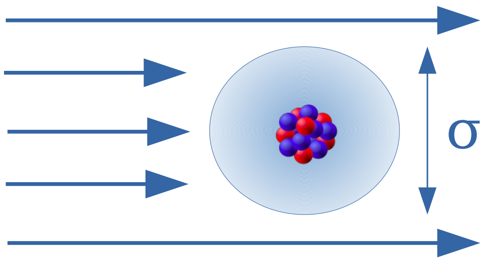
Extension to multiple scattering



Multiple Scattering in Electron Diffraction

Atomic interation cross section

$$P_{scattered} = \sigma\phi_{incident}$$



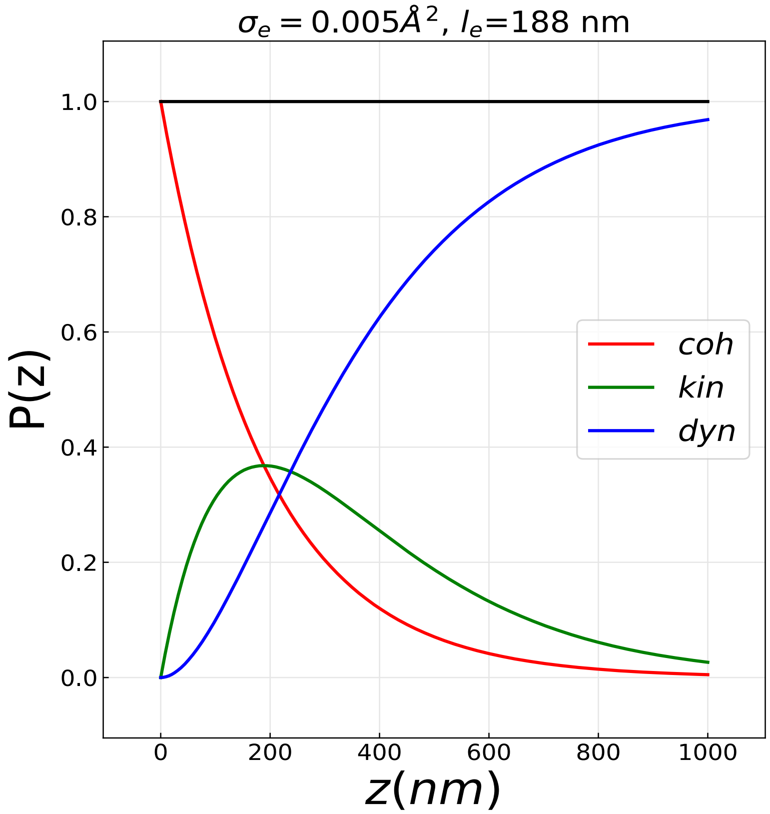
X-rays (Thomson scattering)

$$\sigma_{th} = \frac{8\pi}{3} r_e^2 = 66 fm^2$$

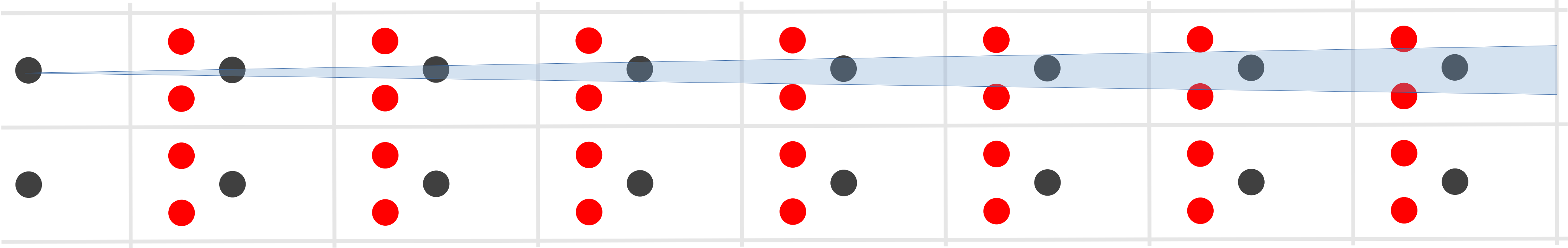
Electrons (Coulomb scattering)

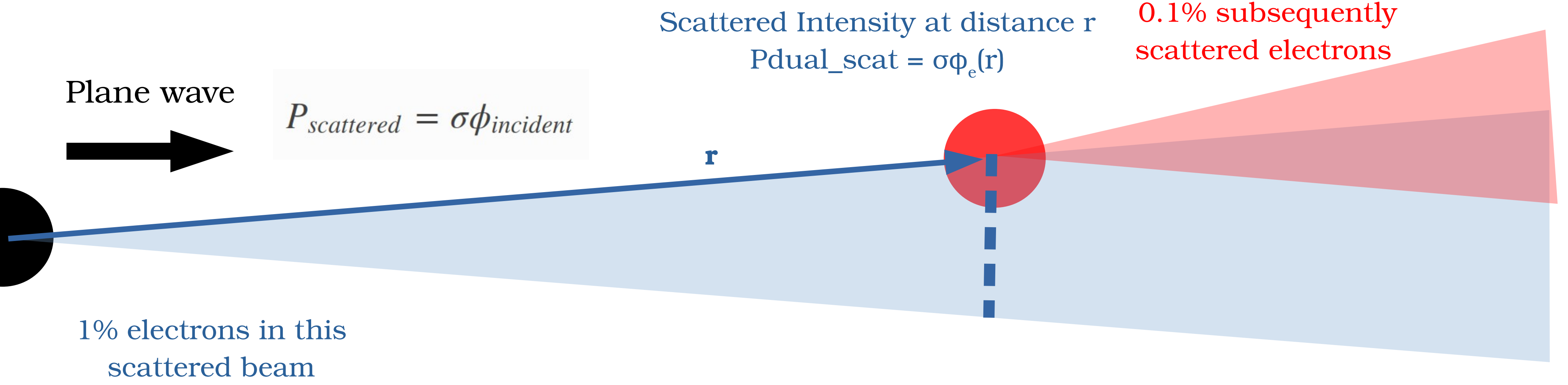
$$\sigma_{th} \approx 1.87 \times 10^6 Z^{4/3} (c/v)^2 = 5 \times 10^7 fm^2$$

Mean free path, l_e = 200nm

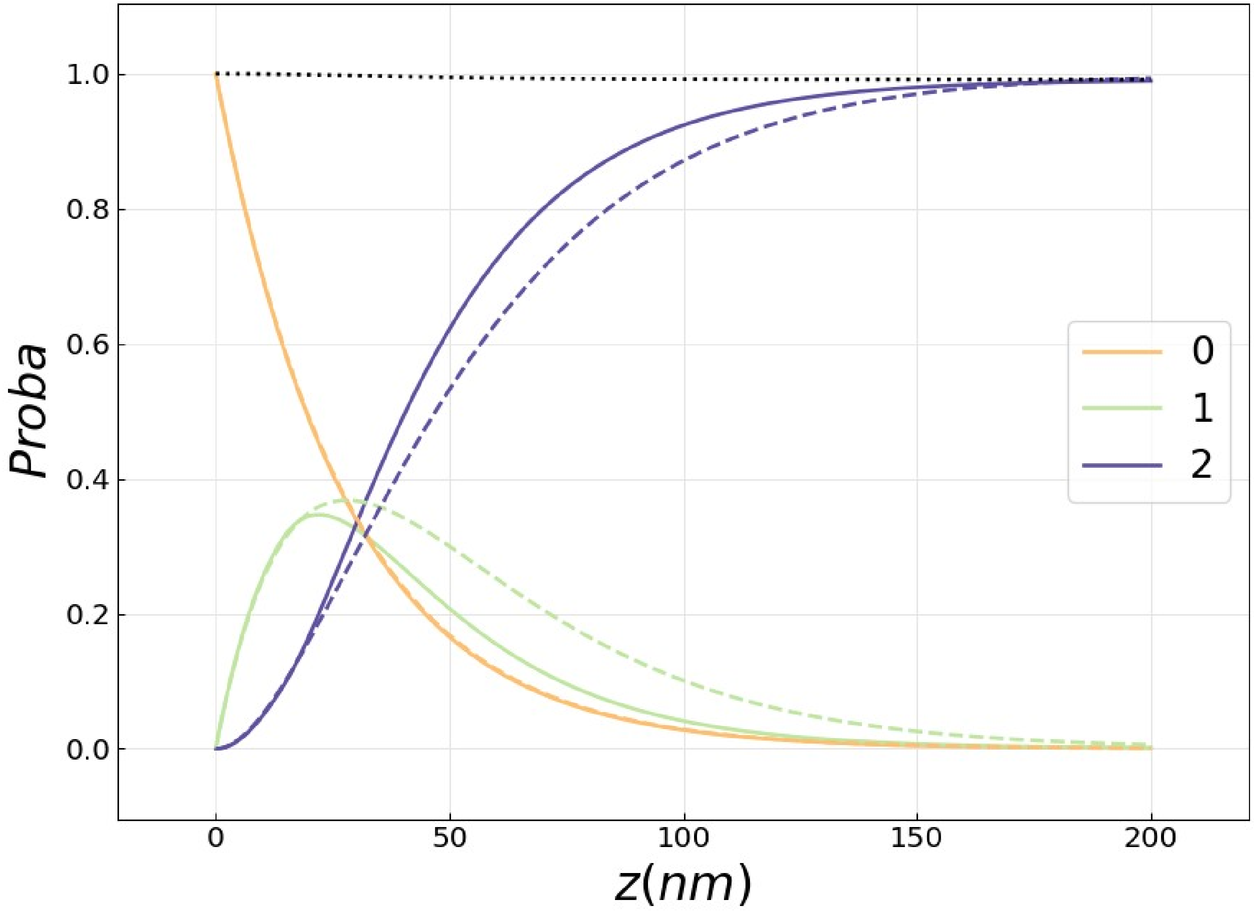


Extension to multiple scattering





Extension to multiple scattering

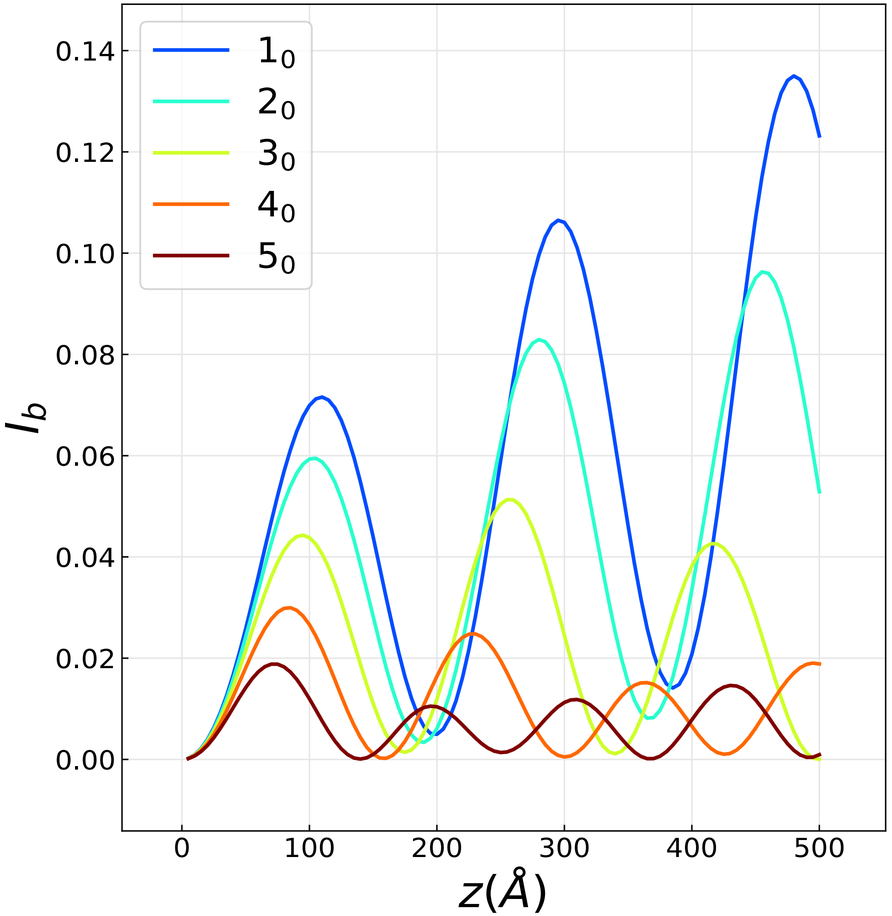


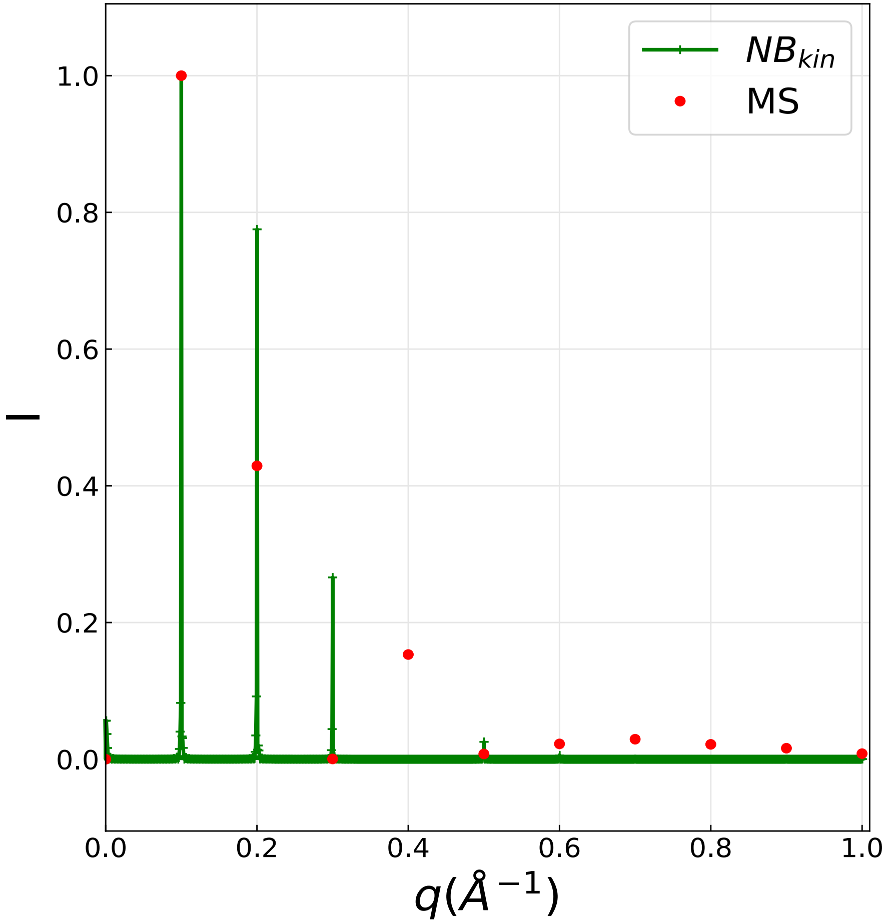
Dashed : near bragg

solid : Theory

0 no scattering
1 single scattering
2 multiple scattering

Near Bragg vs multislice





Current challenges

- adapt nearBragg approach to multiple scattering events

- Compare simluation to experimental dataset

- Simulate defects (modelling and computationnal), Thermal difffuse scattering,

inelastic scattering

- model partially coherent beam as produced by LaB_6 guns