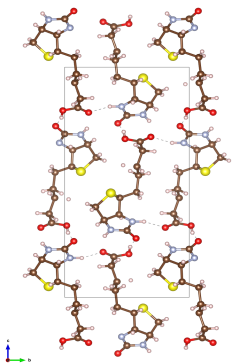
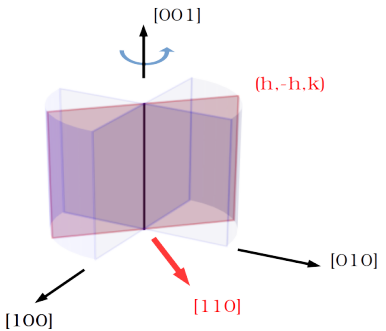
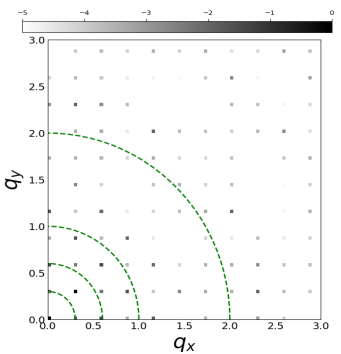
Simulation of Dynamical Scattering Effect in Electron Diffraction Patterns

Tarik Drevon, David Waterman, Eugene Krissinel







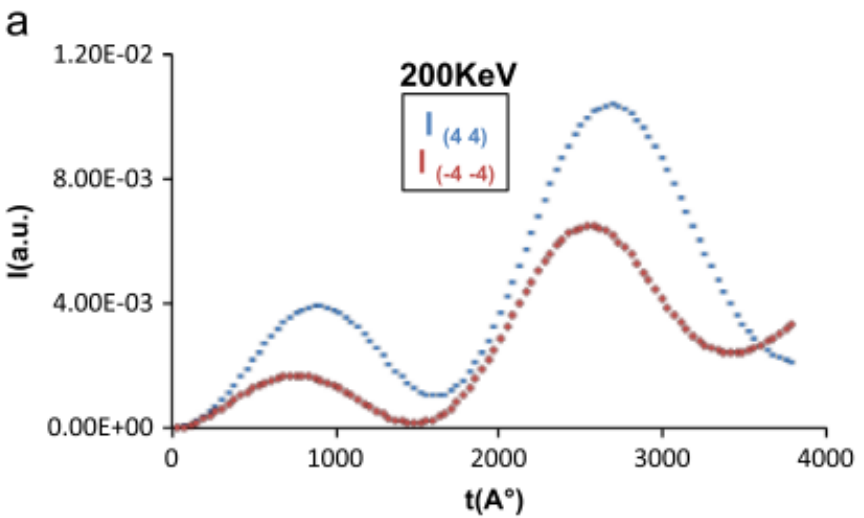
Discrepancy between theory and experiments

Macromolecules solved from experimental Electron Diffraction (ED) data

Sample	Year	Resolution
Lysozyme (14.4 kDa)	2013	2.9 Å
Sup35 prion protein core (905 Da)	2016	1.0 Å
$Au_{146}(p\text{-}MBA)_{57}$ nanoparticle (37.5 kDa)	2017	0.85 Å

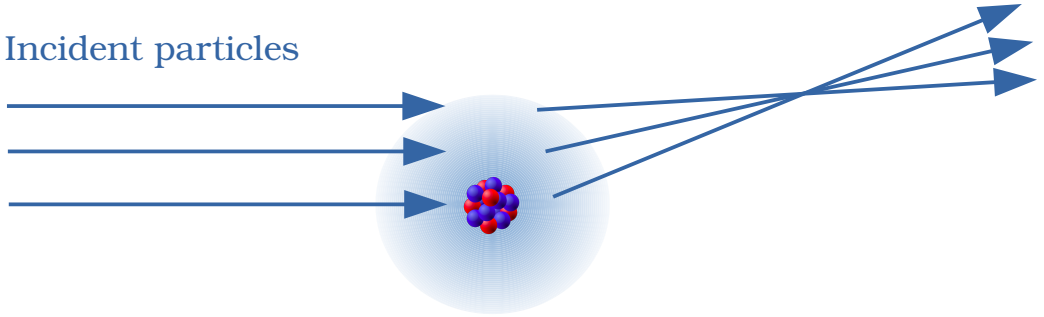
B. L. Nannenga and T. Gonen, "The cryo-EM method microcrystal electron diffraction (MicroED)," Nat. Methods, vol. 16, no. May, pp. 369–379, 2019

Multiple scattering should prevent use of standard X-ray kinematic technique



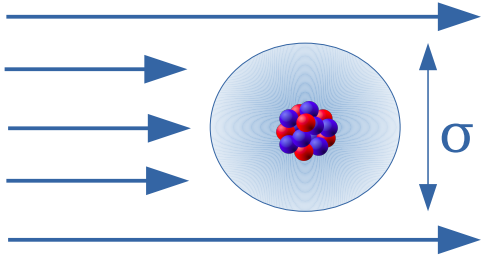
G. Subramanian, S. Basu, H. Liu, J. Zuo, and J. C. H. Spence, "Solving protein nanocrystals by cryo-EM diffraction : Multiple scattering artifacts," Ultramicroscopy, vol. 148, pp. 87–93, 2015

Electron diffraction and dynamical scattering



Atomic interation cross section

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



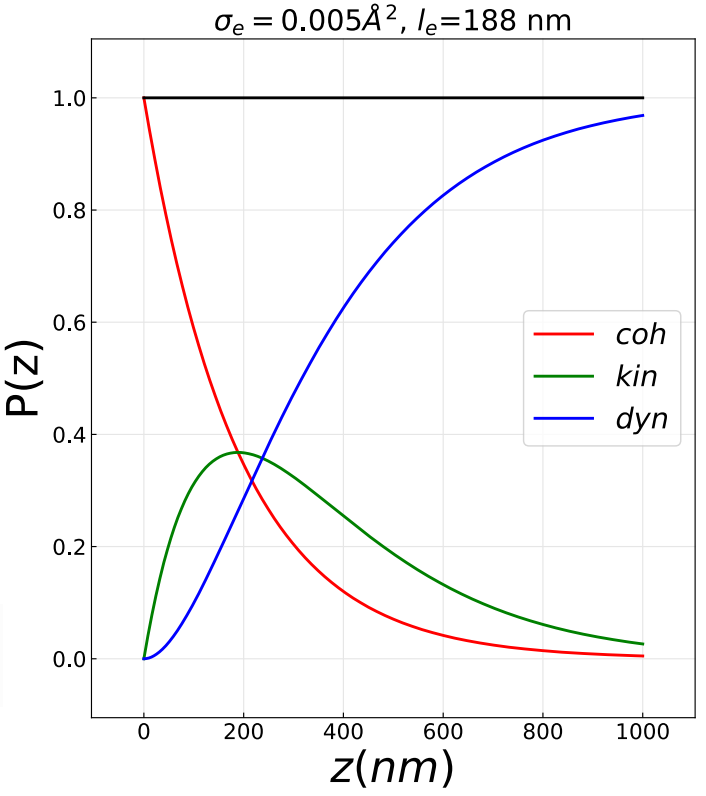
X-rays (Thomson scattering)

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

Electrons (Coulomb scattering)

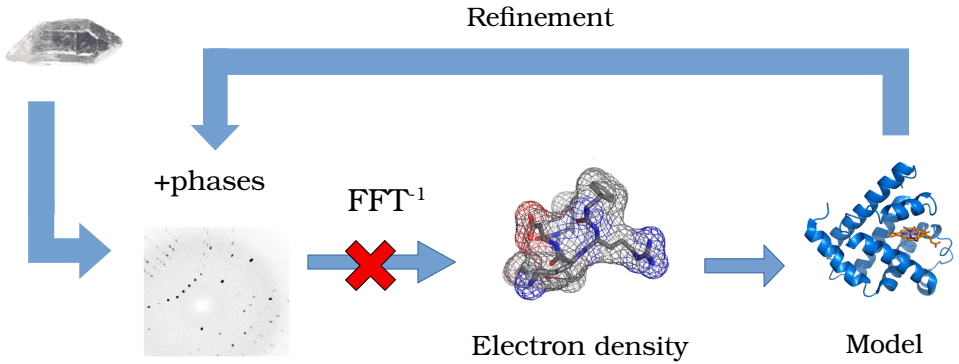
$$\sigma_{th} \approx 1.87 \times 10^6 Z^{4/3} (c/v)^2 = 5 \times 10^7 fm^2$$

Mean free path $l_e = 1/\sigma_e \rho$



Numerical simulation tools of ED patterns

Born approximation (used for X-rays)



Schrodinger's fast electron wave equation

$$\partial_z^2 \ll 2ik_0\partial_z$$

$$\left\{\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r})\right\}\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

$$\frac{\partial\Psi(x,y,z)}{\partial_z} = \left\{\frac{i\lambda}{4\pi}\nabla_{xy}^2 + i\sigma V(x,y,z)\right\}\Psi(x,y,z)$$

Method	Exact/ consistent	Speed	Memory (per atoms)	Periodic structure	Grid based	Package
Multislice (MS) (physical optics based approach)	no	fast	10 points	yes	yes	**TEMSIM (pyMS)** PRISM,…
Bloch wave (diagonalization in reciprocal space)	yes	slow	10 points	yes	no	EDM,PyQt,…
Near bragg (real space path differences)	no	??	1 point	no	no	NearBragg (James Holton)

Multislice algorithm (MS)

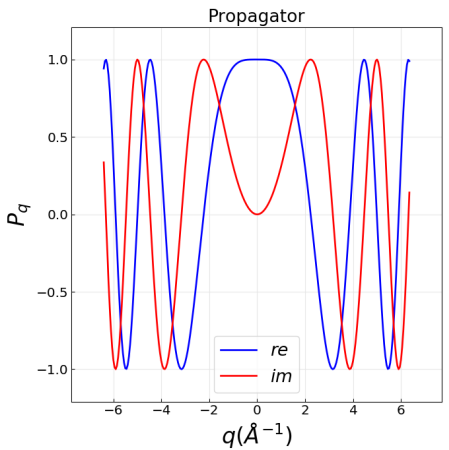
$$\frac{\partial \Psi(x,y,z)}{\partial_z} = \left\{ \frac{i\lambda}{4\pi} \nabla^2_{xy} + i\sigma V(x,y,z) \right\} \Psi(x,y,z)$$

FFT

$$\Psi(z+\Delta z) = p(x,y,\Delta z) * \Big(t(x,y,z)\Psi(z) \Big)$$

Fresnel propagator

$$p(x,y,\Delta z) = \frac{1}{i\lambda \Delta z} e^{ik_0 \frac{x^2+y^2}{2\Delta z}}$$



Transmission function

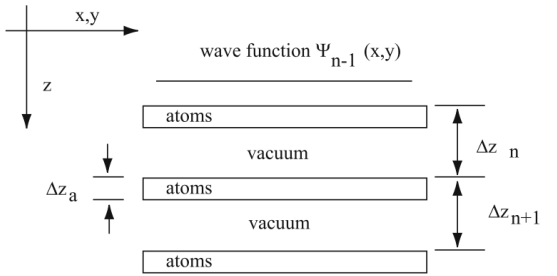
$$t(x,y,z) = e^{i\sigma \nu_{\Delta z}}$$

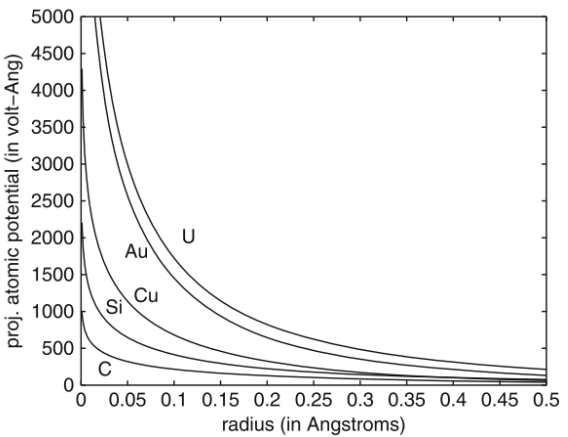
$$\approx 1 + i\sigma \nu_{\Delta z}$$

Weak potential

Projected potential

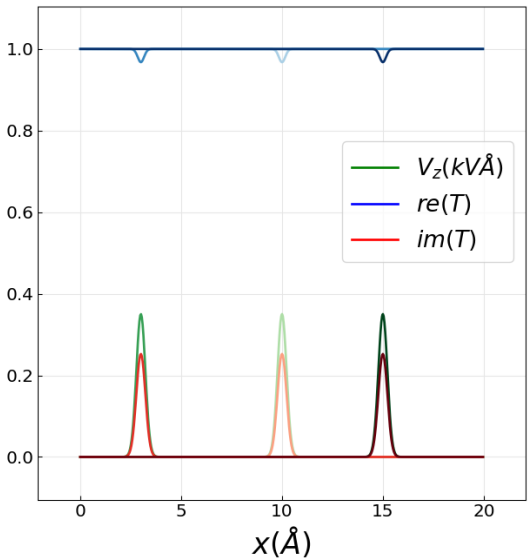
$$\nu_{\Delta_z} = \int_z^{z+\Delta z} V(x,y,z')dz'$$



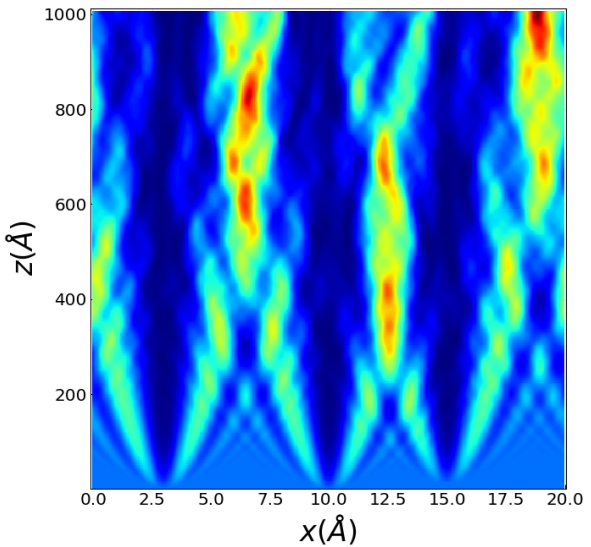


Multislice simple example

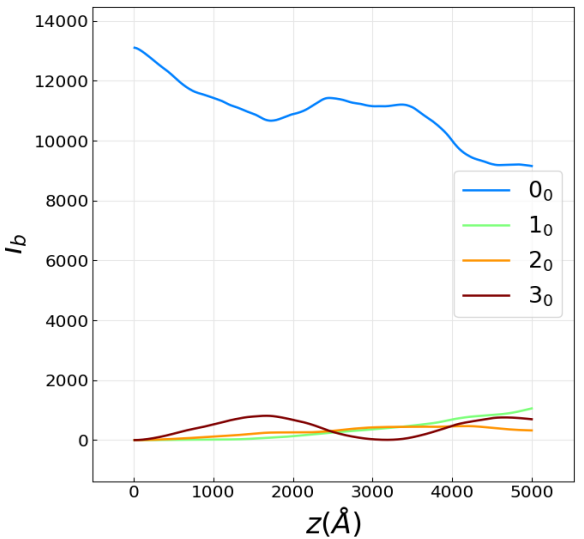
Transmission function and projected potential



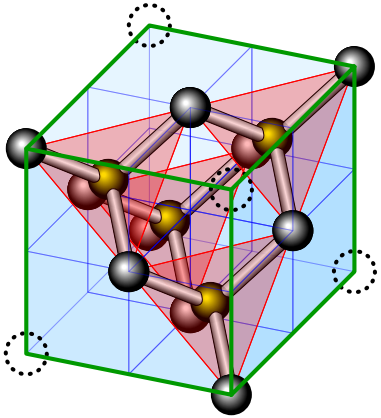
Real space wave function as function of propagation



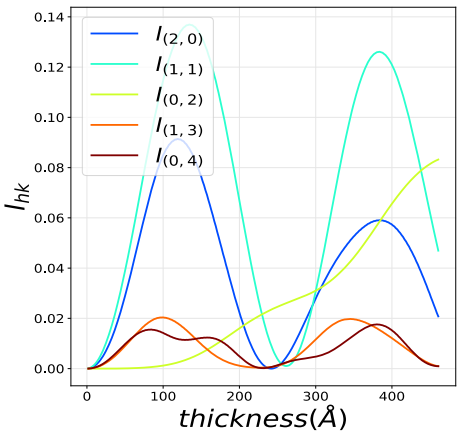
Major beams intensities in reciprocal space

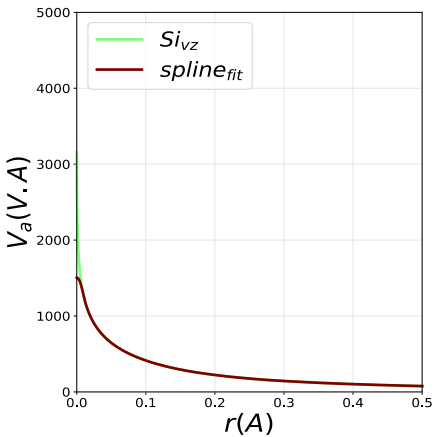


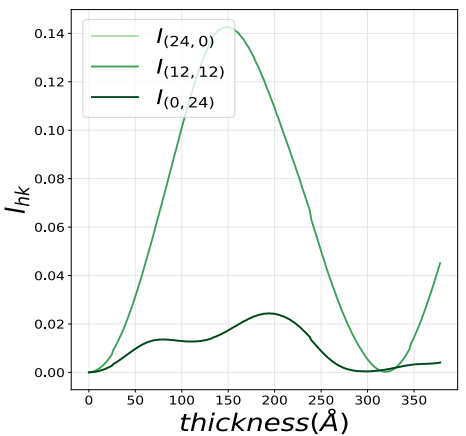
Multislice Silicon Diamond Structure

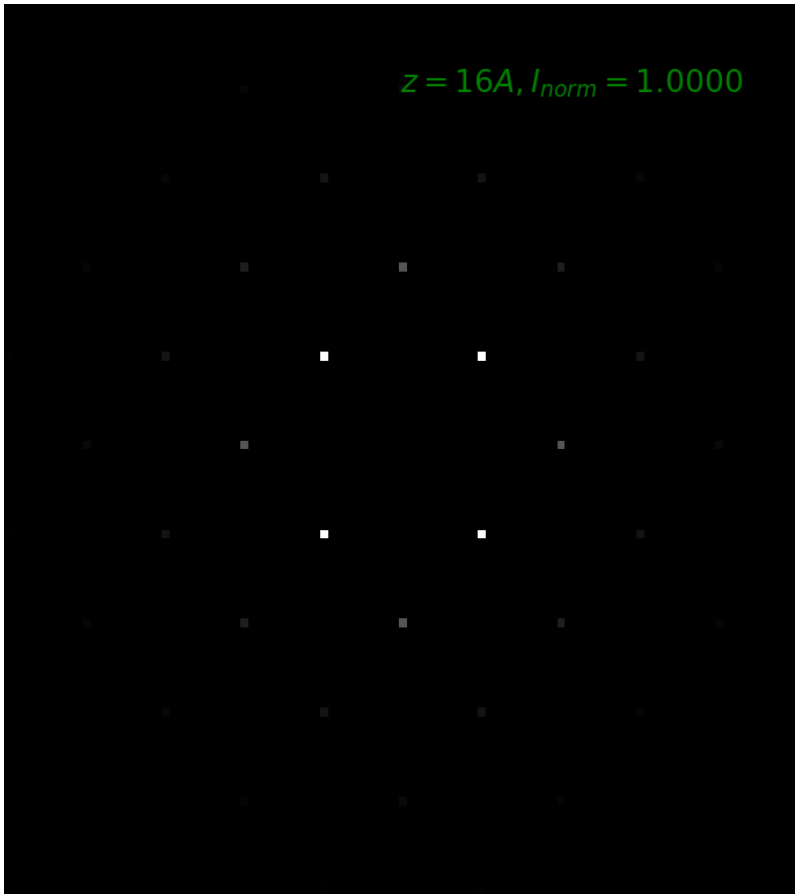


[110] vs [100]





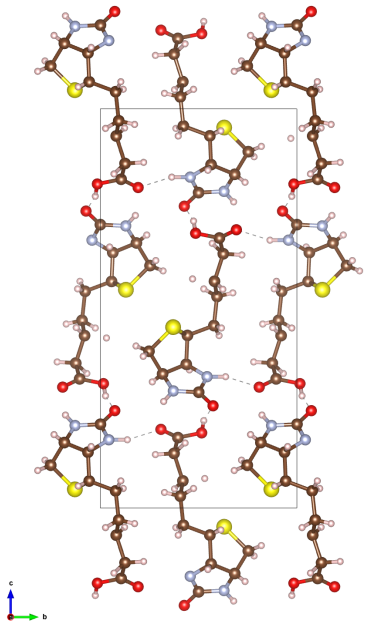




Simulation of biotin $C_{10}H_{16}N_2O_3S$

Structure $P2_12_12_1$

$a = 5.24A,$
$b = 10.35A,$
$c = 21.04A$



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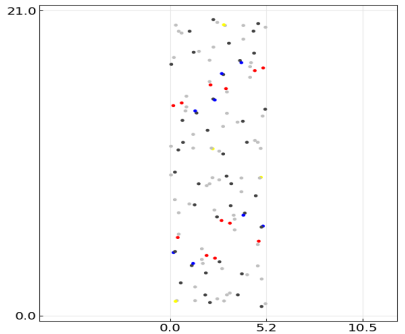

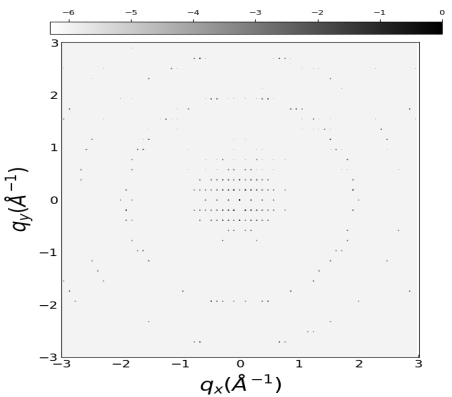

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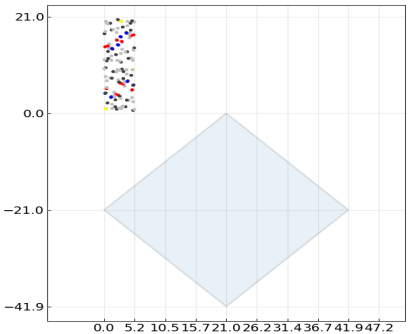

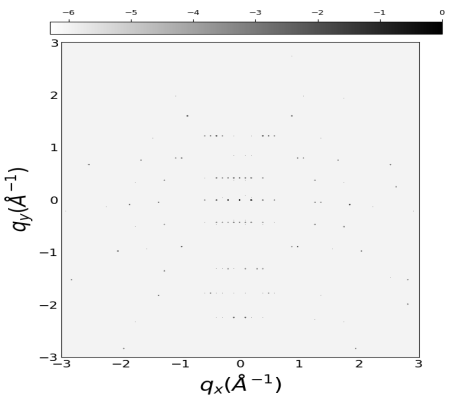

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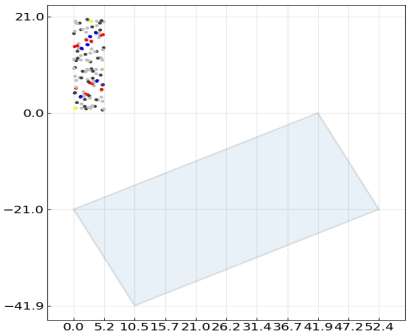

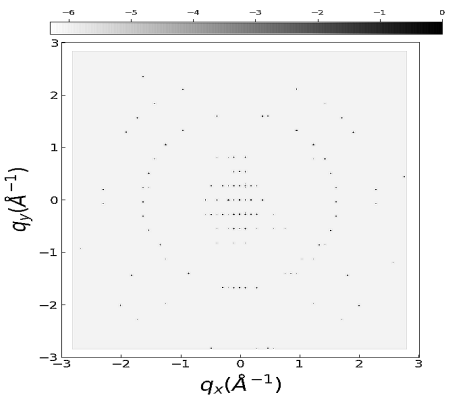

What's next?

- *Use CCP4 with the simulated data*

- *Include effects of defects and solvent scattering*

- *Develop nearBragg approach*

- *Make python interface available from the python index pypi*

More info *http://brno.rc-harwell.ac.uk:8000/* *RCaH VPN required*