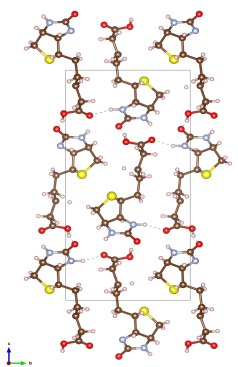
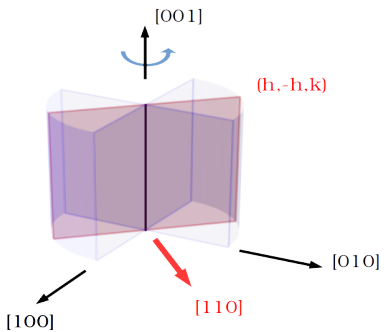
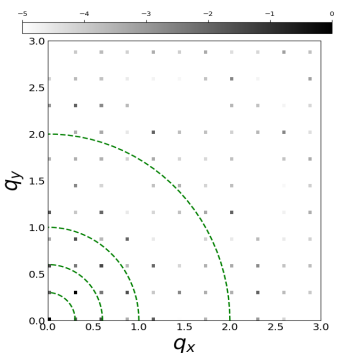
Simulation of Dynamical Scattering in Electron Diffraction Patterns

Tarik Drevon, David Waterman, Eugene Krissinel







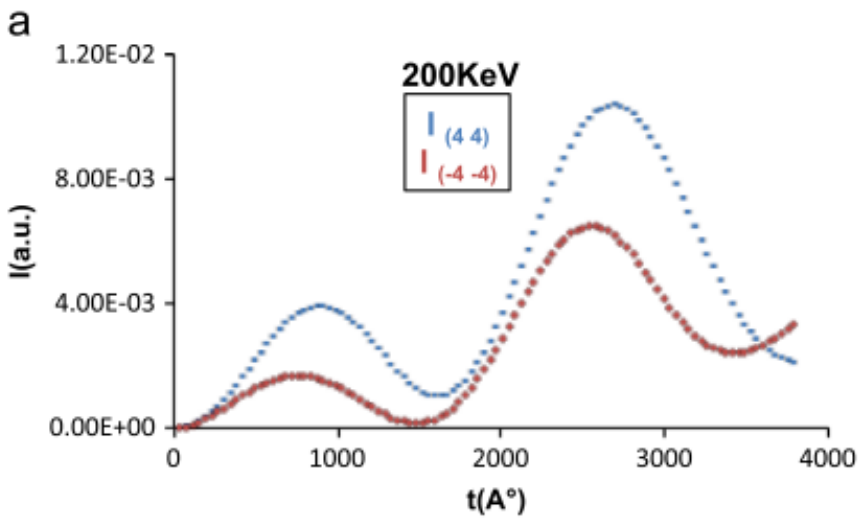
Discrepancy between theory and experiments

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

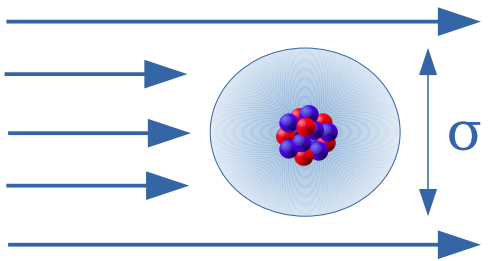


G. Subramanian, S. Basu, H. Liu, J. Zuo, and J. C. H. Spence, "Solving protein nanocrystals by cryo-EM diffraction : Multiple scattering artifacts," Ultramicroscopy, vol. 148, pp. 87–93, 2015

Electron diffraction and dynamical scattering

Atomic interation cross section

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



X-rays (Thomson scattering)

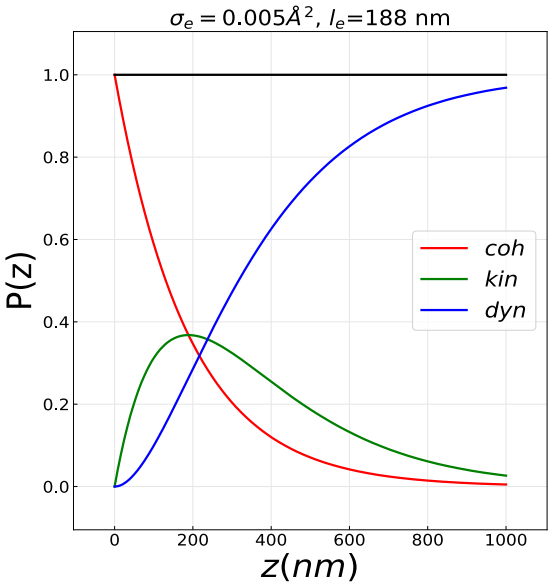
$$\sigma_{th} = \frac{8\pi}{3} r_e^2 = 66 fm^2$$

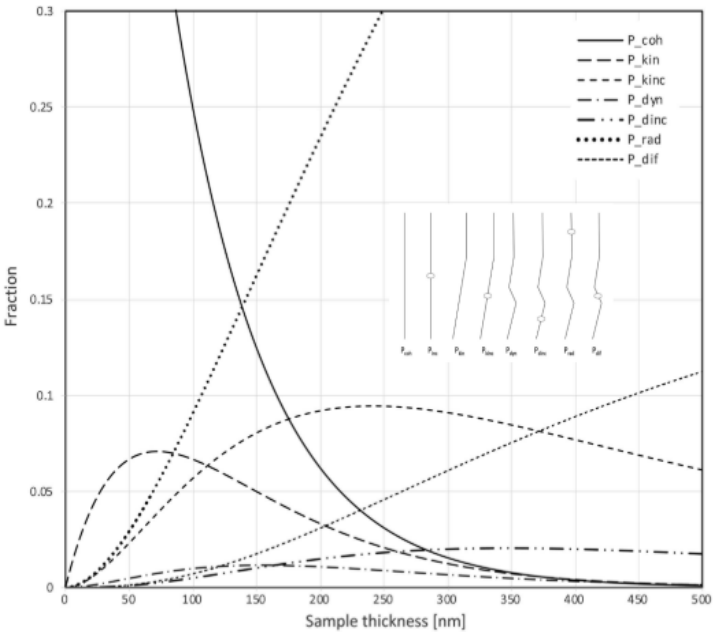
Electrons (Coulomb scattering)

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

Mean free path

l_e = 200nm

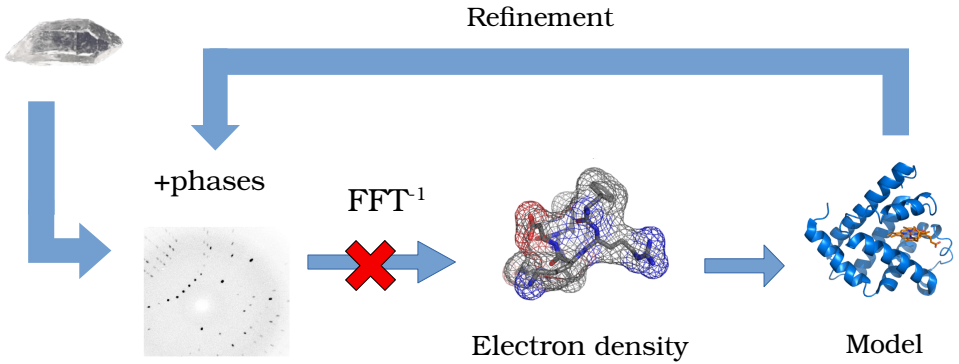




T. Latychevskaia and J. P. Abrahams, "Inelastic scattering and solvent scattering reduce dynamical diffraction in biological crystals," Acta Crystallogr. Sect. B Struct. Sci. Cryst. Eng. Mater., vol. 75, pp. 523–531, 2019

Numerical simulation tools of ED patterns

Born approximation (used for X-rays)

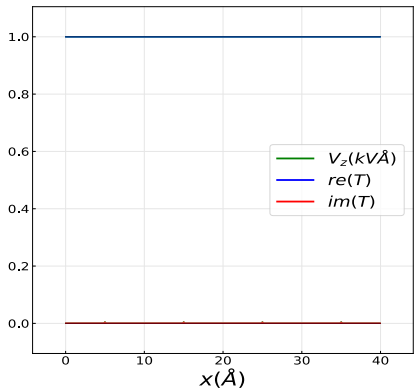
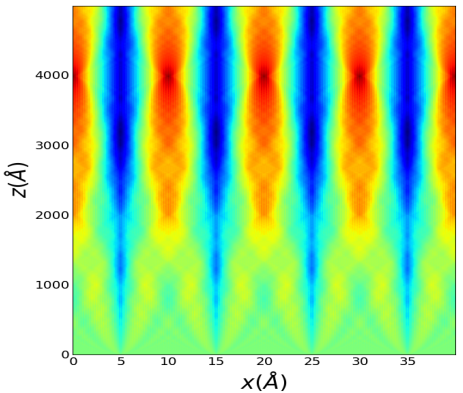
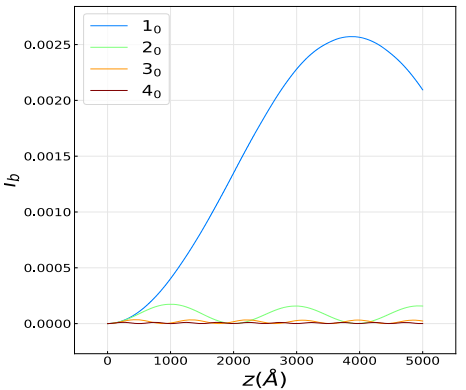
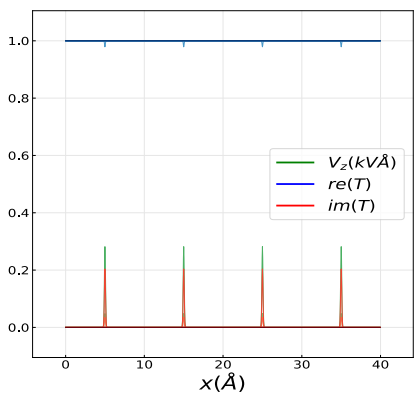
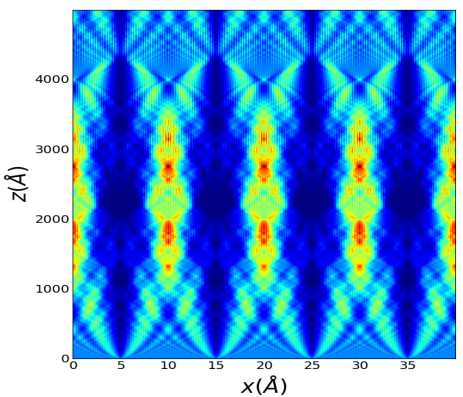
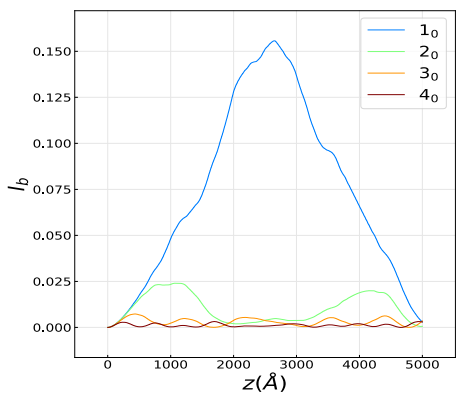


Schrodinger's fast electron wave equation

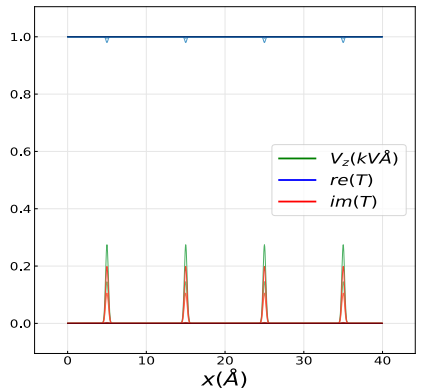
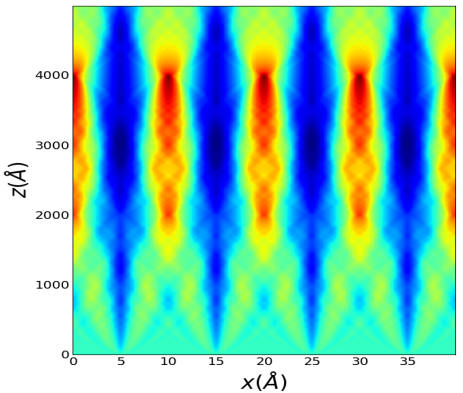
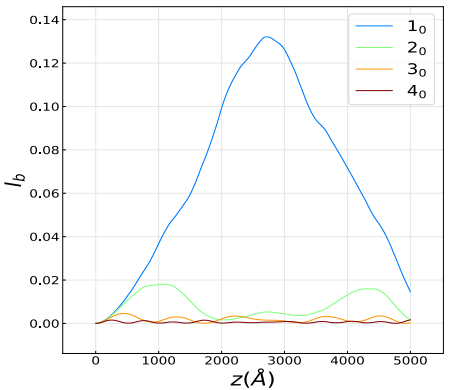
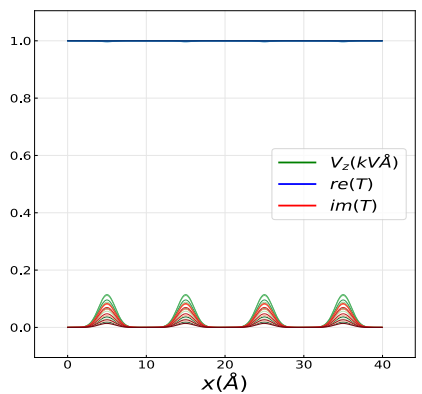
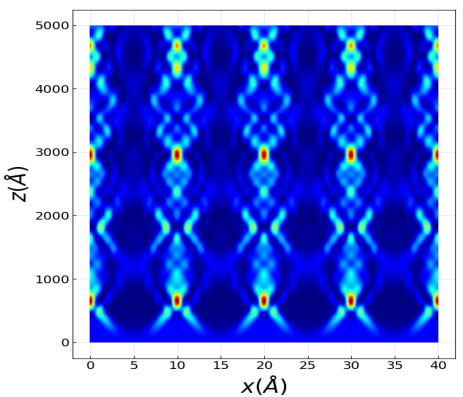
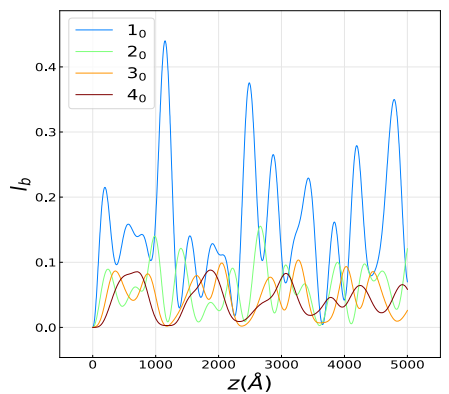
$$\frac{\partial \Psi(x,y,z)}{\partial_z} = \left\{ \frac{i\lambda}{4\pi} \nabla^2_{xy} + i\sigma V(x,y,z) \right\} \Psi(x,y,z)$$

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)

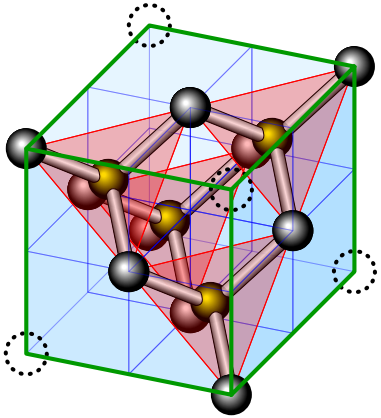
Multislice 2D examples : electrostatic potential

Potential strength	Transmission function and projected potential	Wave function inside the crystal	Beams intensities in Reciprocal space
Weak			
Strong			

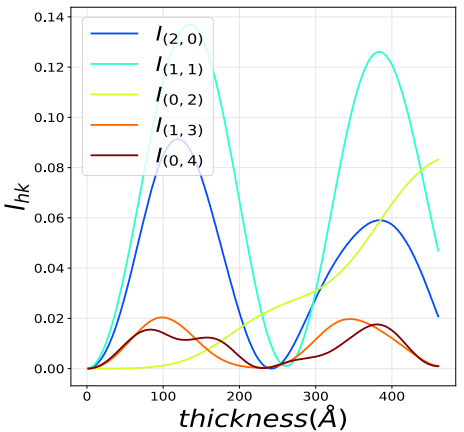
Multislice 2D examples : electrostatic potential

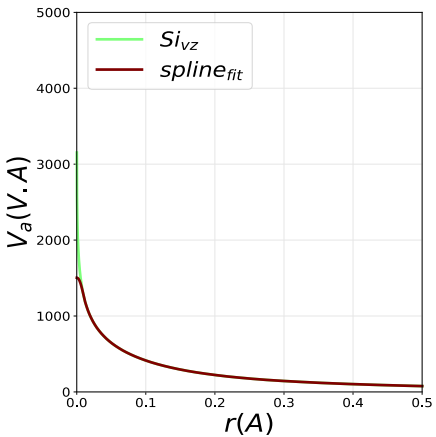
Potential	Transmission function and projected potential	Wave function inside the crystal	Beams intensities in Reciprocal space
small atomic overlap			
large atomic overlap			

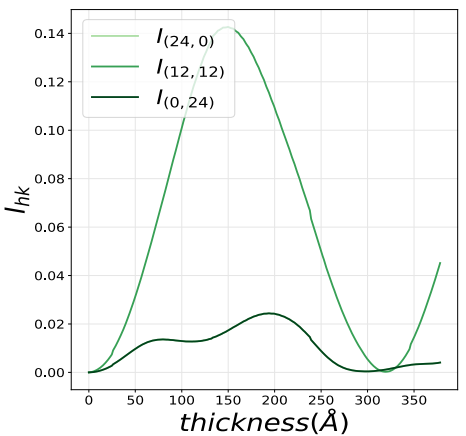
Multislice Silicon Diamond Structure

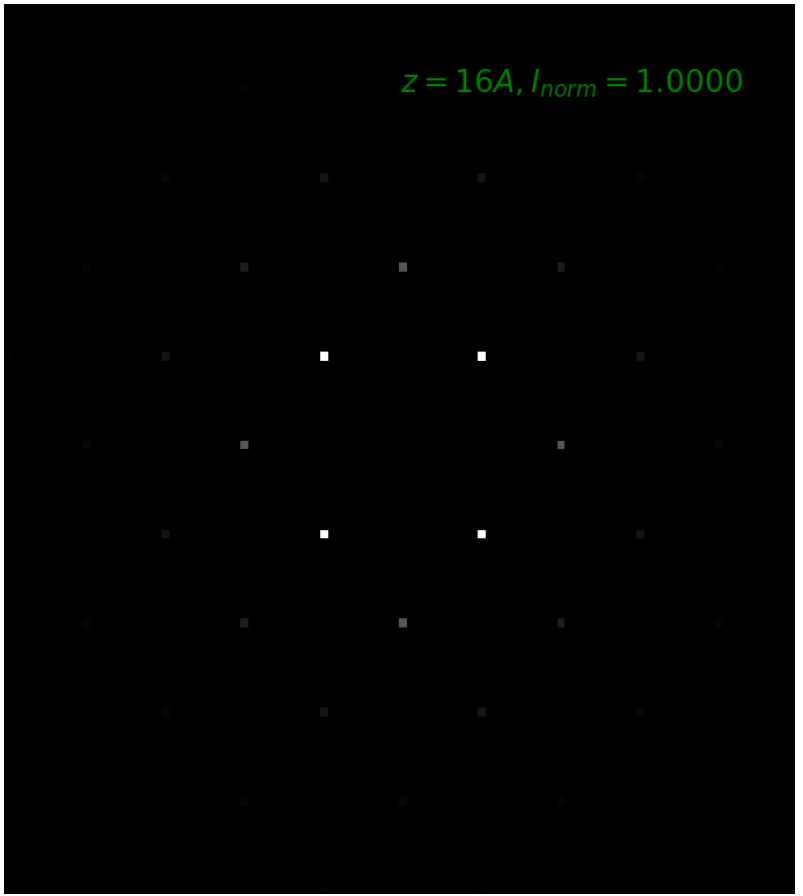


[110] vs [100]





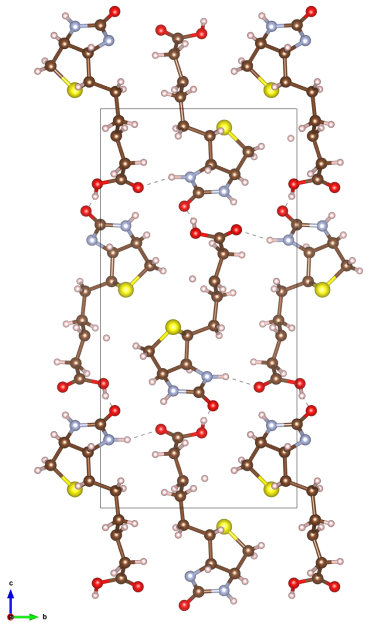




Simulation of biotin $C_{10}H_{16}N_2O_3S$

Structure $P2_12_12_1$

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



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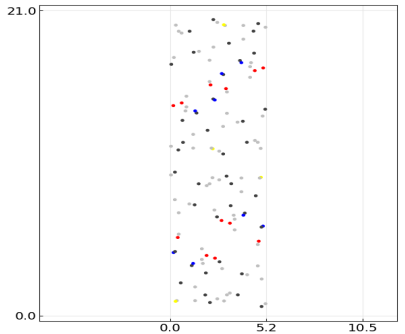

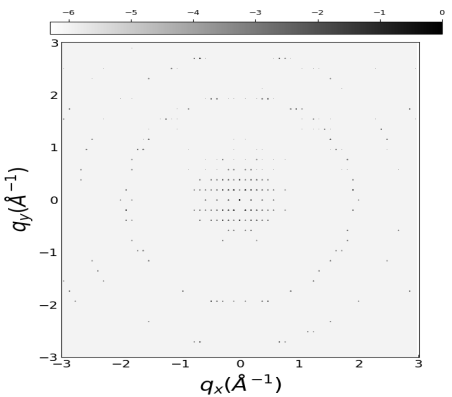

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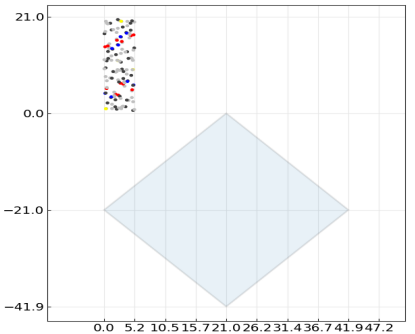

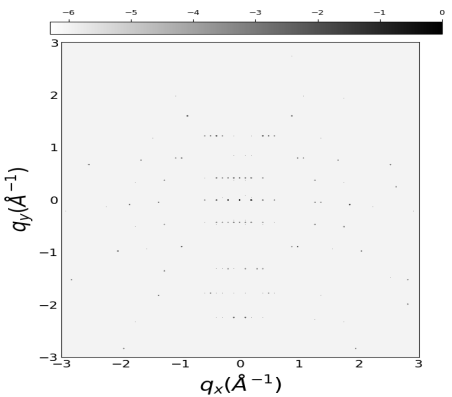

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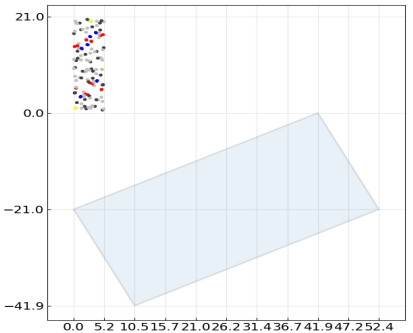

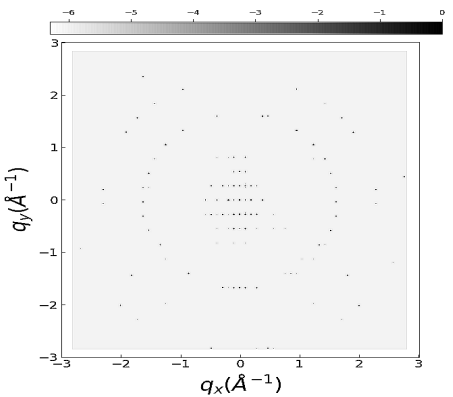

What's next?

- *Use CCP4 with the simulated data*

- *Investigate effect of defects, solvent, inelastic scattering*

- *Further develop nearBragg approach*

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

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