Virtual Beamline Meets CHX Commissioning

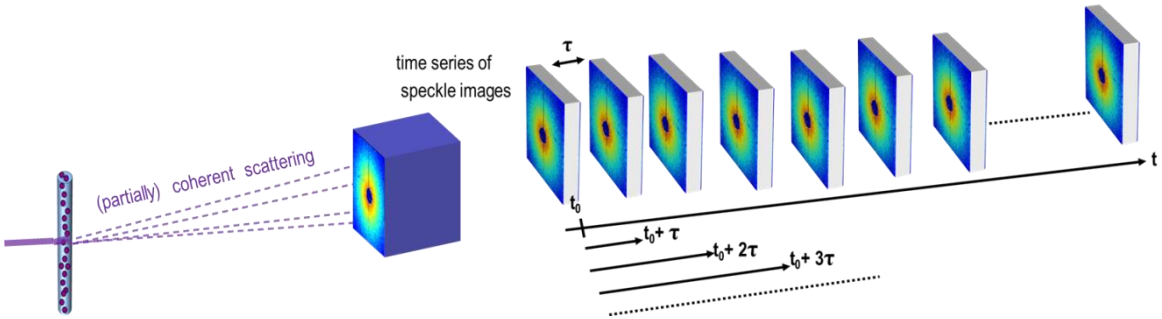
Collaboration Meeting on "Simulation and Modeling for SR Sources and X-Ray Optics", *2 October 2015*

Outline

- Introduction to the Coherent Hard X-ray Scattering beamline
- Wavefront propagation simulations with SRW
- CHX commissioning results evaluated by SRW simulations
- Beyond beamline comissioning
- Summary and conclusions

Introduction: Scientific Mission of the CHX beamline

The CHX beamline is optimized for time-resolved coherent scattering experiments, such as X-ray photon correlation spectroscopy (XPCS) over a large (simultaneous) Q-range

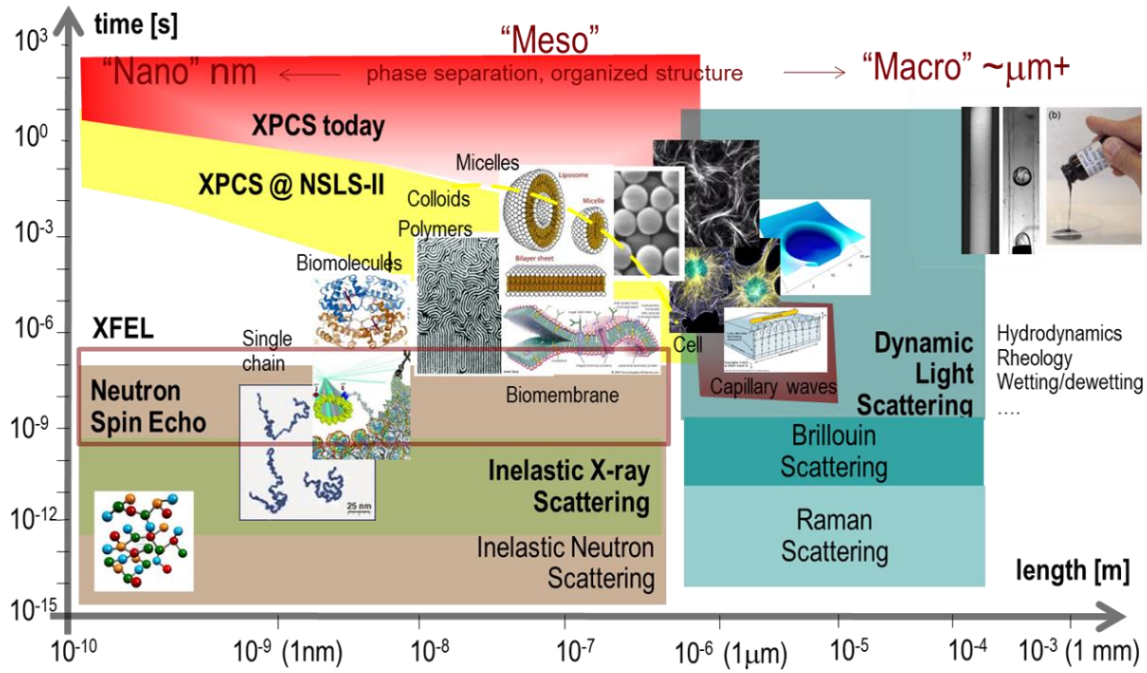


- resolving dynamics by time-resolved coherent scattering
- other 'flavors', such as speckle visibility spectroscopy

- flux determines accessible time scales
- degree of coherence determines 'contrast' in the correlation functions

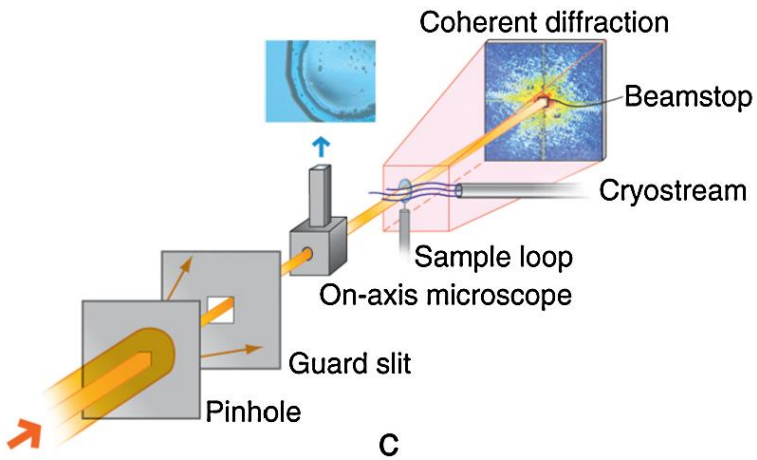
targeting nano - mesoscale length scales and dynamics with time scales ≥μs, such as:

- colloidal glasses
- polymers
- bio-membranes

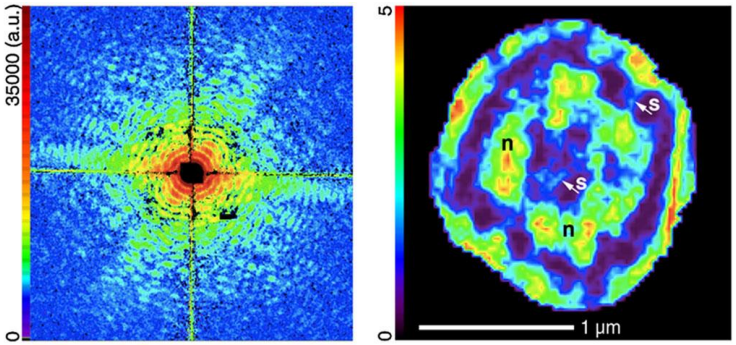


Introduction: Scientific Mission of the CHX beamline

Capabilities beyond base-scope: (full-field) coherent diffraction imaging

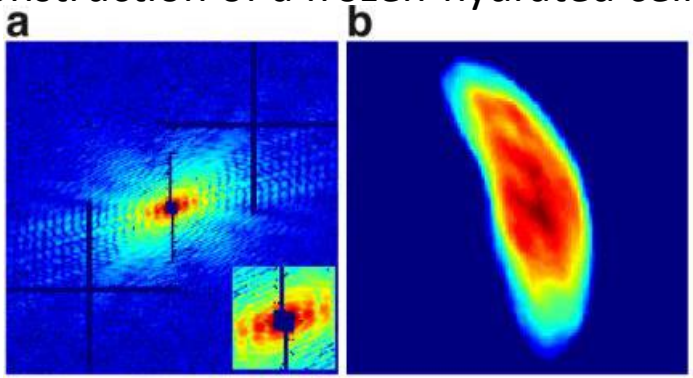


2D reconstruction of a frozen-hydrated bacteria

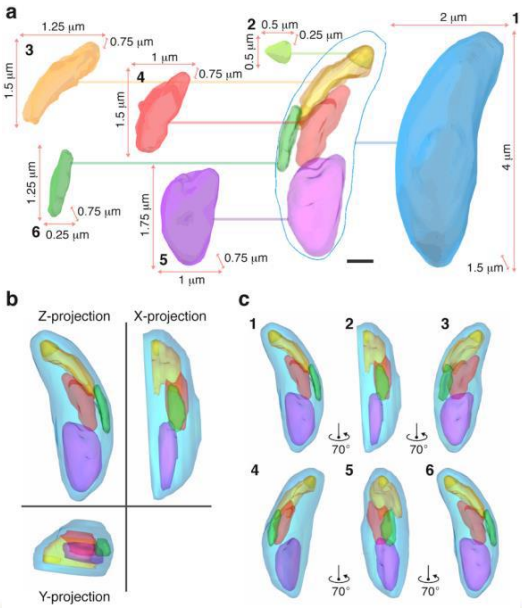


E. Lima *et al.*, PRL (2009)

3D reconstruction of a frozen-hydrated cell



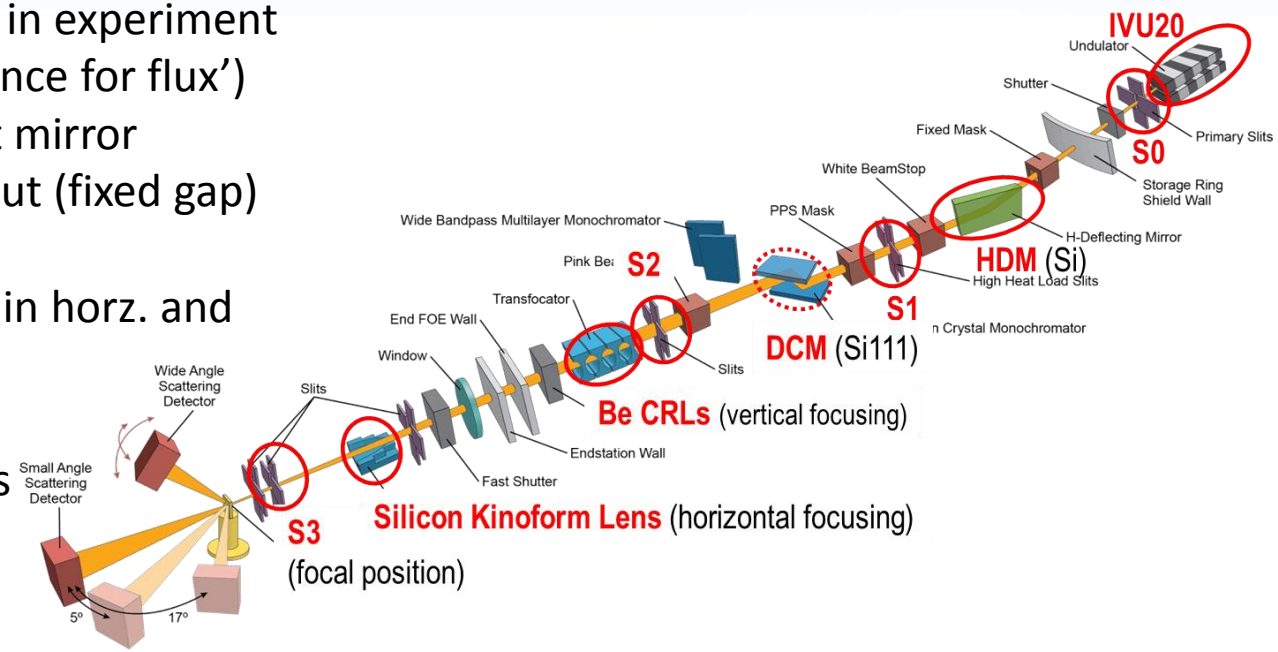
J. A. Rodriguez *et al.*, IUCrJ (2015)



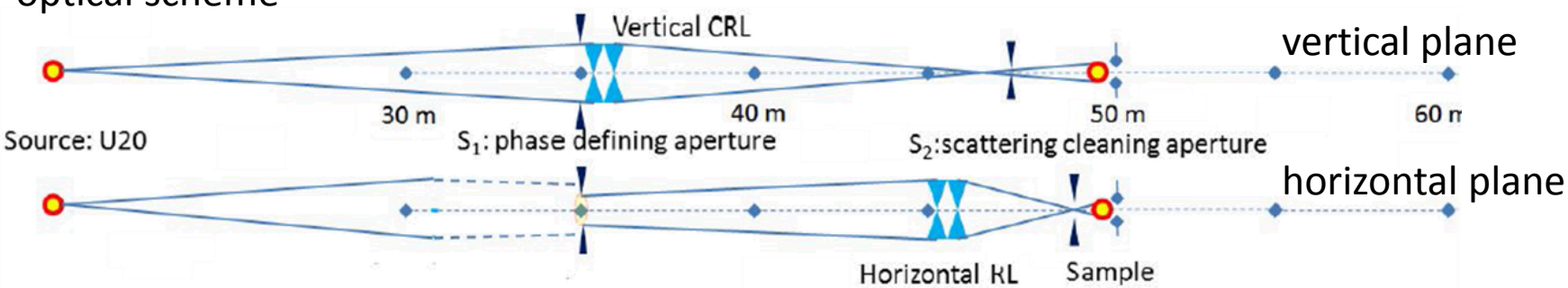
- typically requires higher degree of coherence
- flux related to achievable resolution

Introduction: Layout coherent SAXS / full-field CDI

- control phase space used in experiment with S2 slit (trade 'coherence for flux')
- horizontally reflecting flat mirror
- vertical pseudo-channel cut (fixed gap) DCM
- independent 1D focusing in horz. and vert.:
  - vert.: Be CRLs
  - horz.: Si kinoform lenses



optical scheme



O. Chubar *et al.*, Journal of Physics, Conf. Ser., 425 (2013)

Introduction: Wavefront Propagation Simulations (a user's prospective)

- All techniques at CHX exploit the partial coherence of the source -> need a wave based description of the beamline, preferably one that can be operated as a 'user'

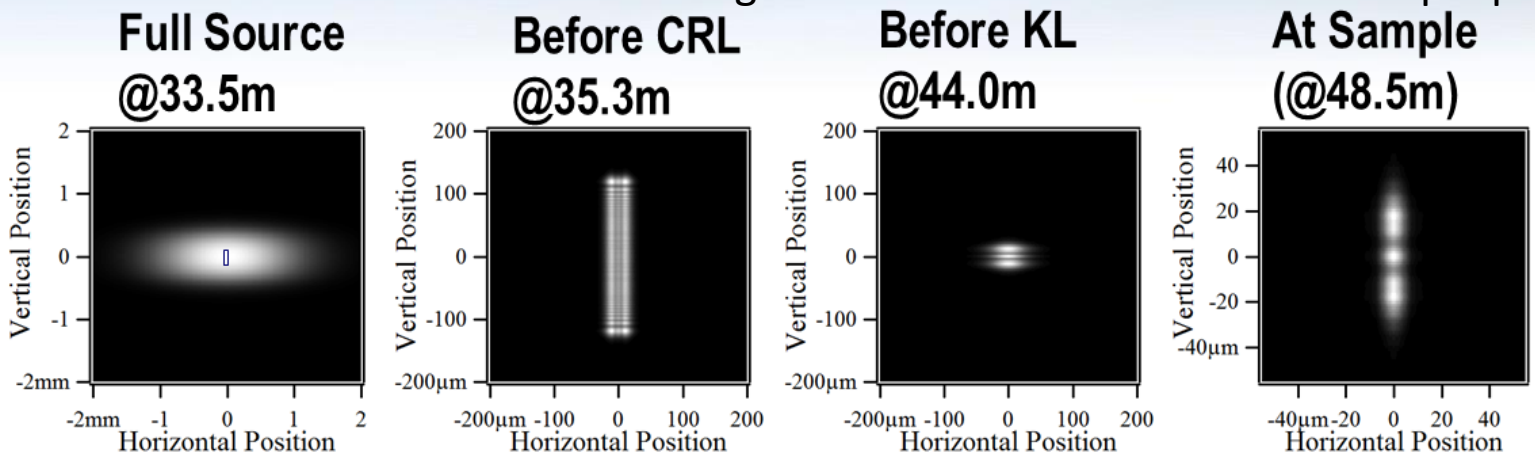
- Wavefront propagation simulations in the 'Synchrotron Radiation Workshop' (SRW) software package [O.Chubar and P.Elleaume, *Proc. EPAC-98*, 1177-1179 (1998)] capture the effects of partial coherence

- multi-electron simulations: sum of propagated (fully coherent) single electron emission with different parameters form the allowed electron phase space

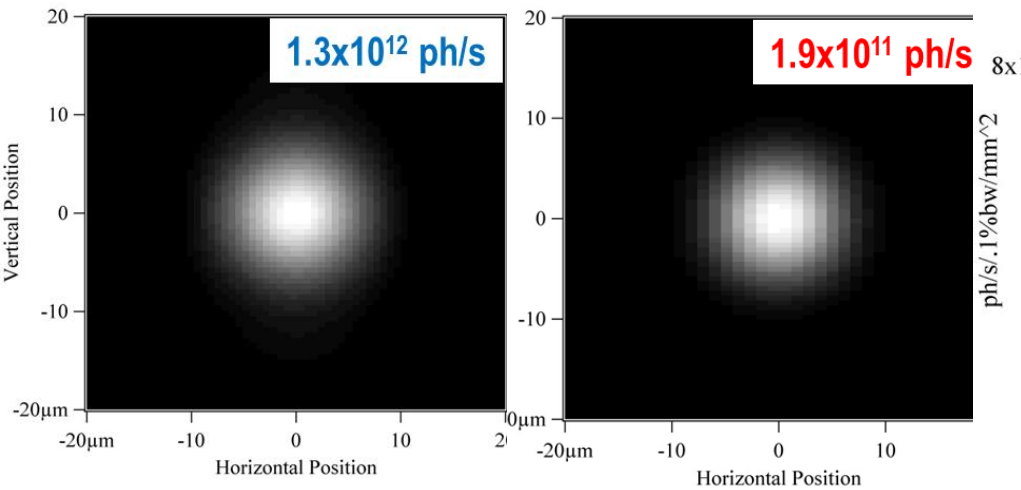
- Wavefront propagation simulations are used for:
  - beamline design ☑
  - simulation assisted commissioning ☐
  - simulation of experimental data ☐
  - interpretation / improvement of collected data by solving inverse problems ☐

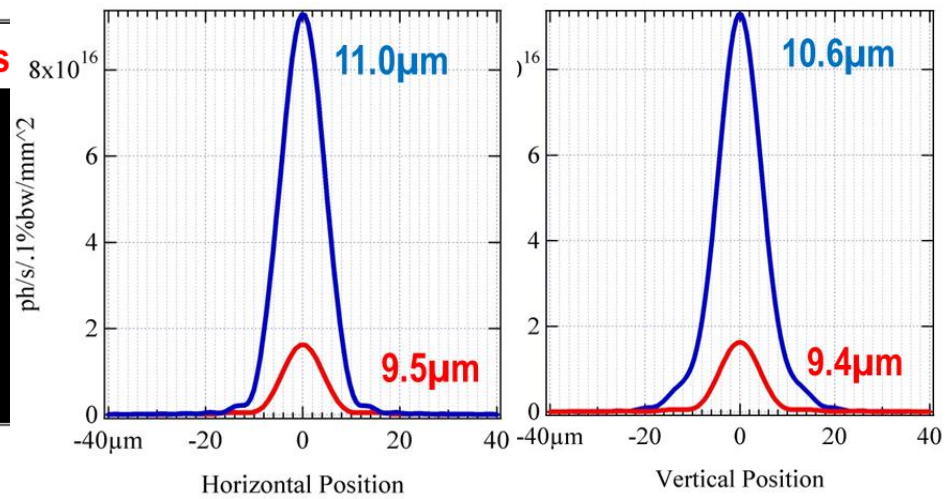
SRW simulations for beamline design

simulations of beam size and flux throughout the beamline and at the sample position (9keV)



specific gap of S2 causes beam splitting



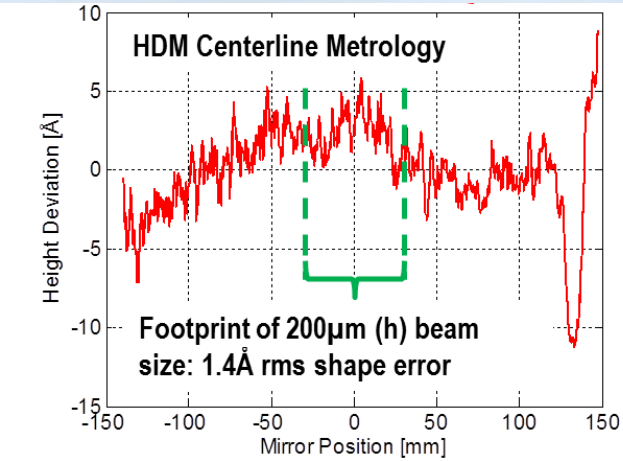


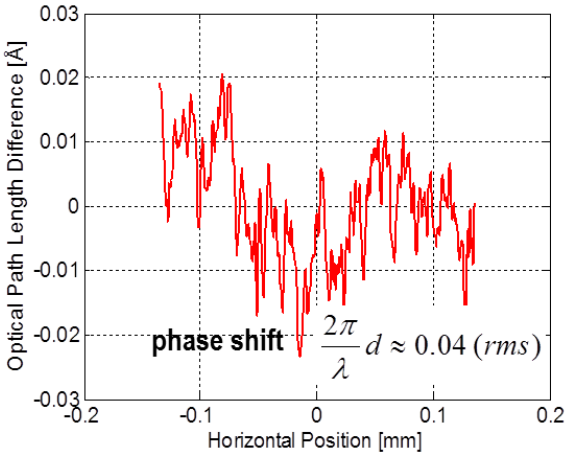
S0: 0.2(h)x1.0(v)mm^2; S1: 0.2(h)x1.0(v)mm^2;
S2: 0.05(h)x0.2(v)mm^2; S3: 0.01(h)x0.01(v)mm^2

S0: 0.3(h)x1.0(v)mm^2; S1: 0.3(h)x1.0(v)mm^2;
S2: 0.1(h)x1.0(v)mm^2; S3: 0.02(h)x0.02(v)mm^2

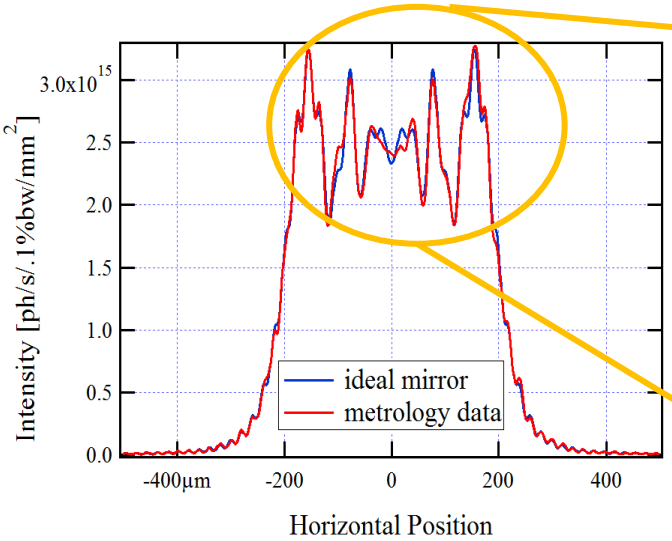
SRW simulations for beamline design

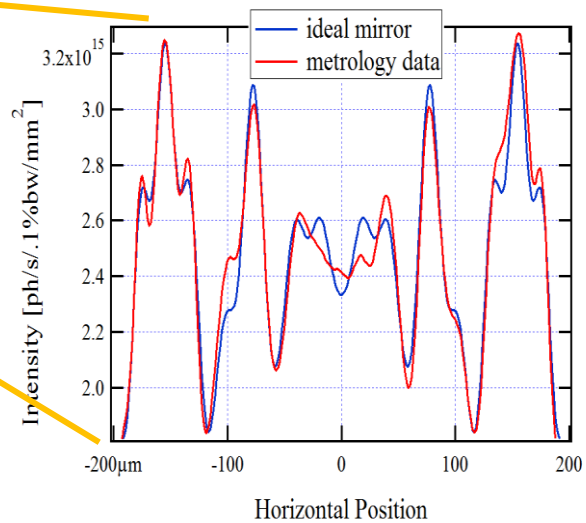
- effect of 'imperfect' HDM
- metrology data from mirror supplier (JTech)
- virtually no influence in the partial coherent regime, due to excellent mirror quality and horizontal geometry



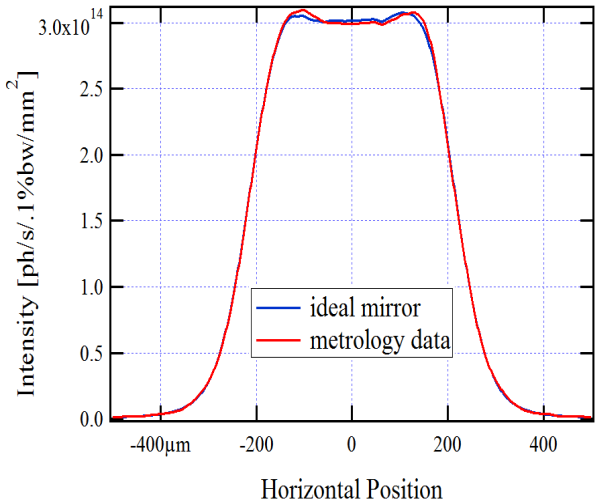


single electron emission @sample



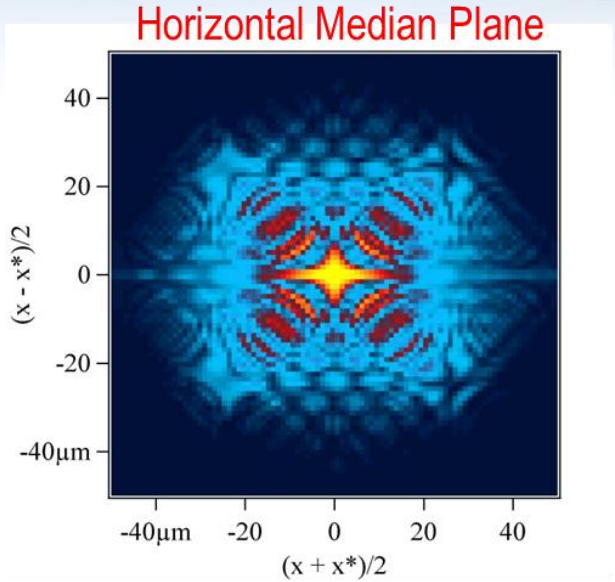


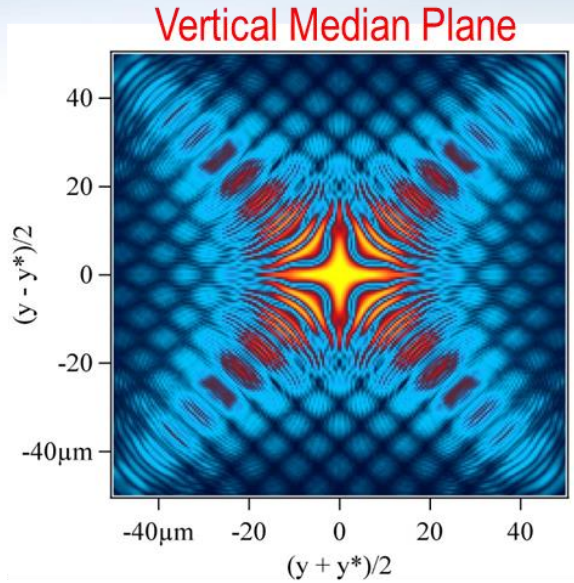
multi electron emission @sample



SRW simulations for beamline design

simulation of mutual intensity -> transverse coherence lengths





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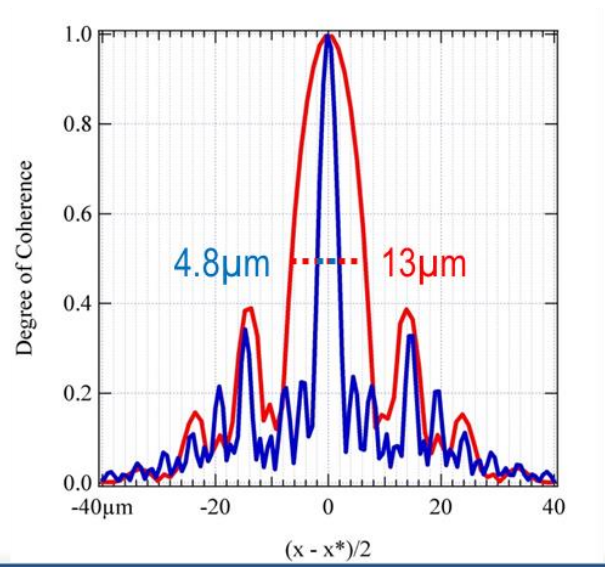
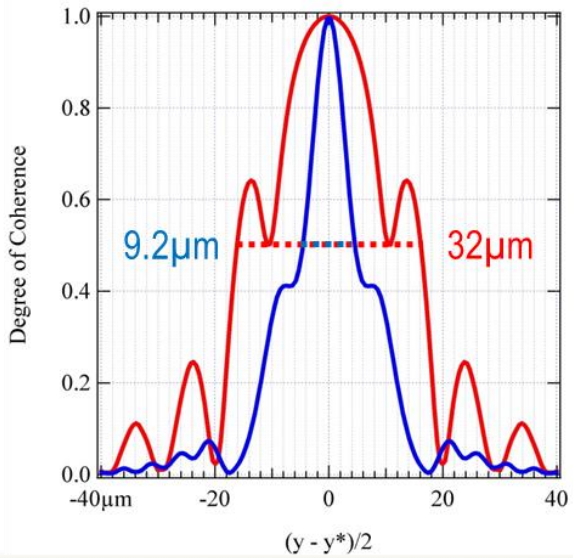
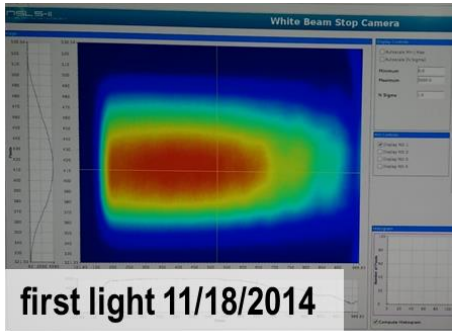




Wavefront Propagation Simulation: meeting reality

Commissioning of the Coherent Hard X-ray beamline at NSLS-II started in Nov. 2014

Not all capabilities are currently installed, e.g. point detectors, horizontal focusing,….will be installed over the summer -> cannot measure final performance parameters / perform measurements in an 'ideal' way

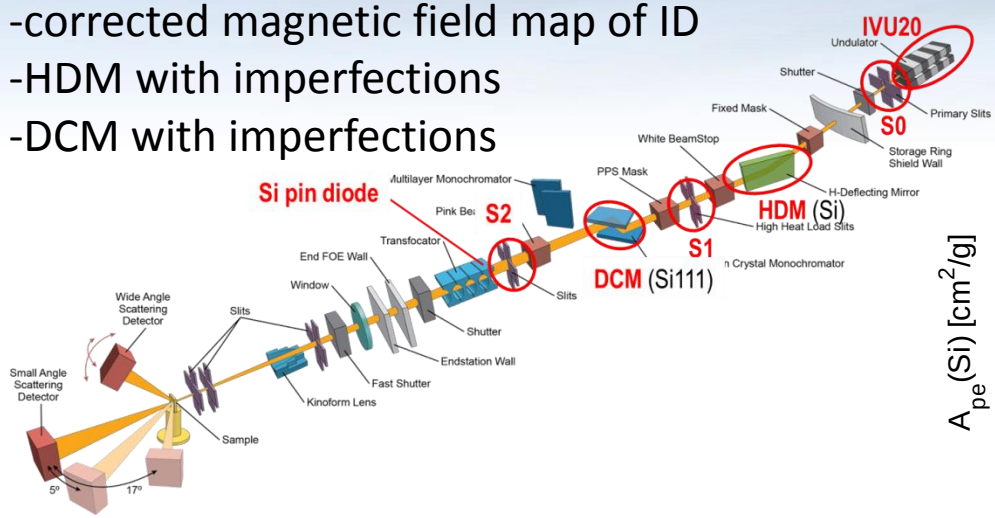


⇒ measure beam parameters, such as flux, vertical focus, coherence,… with currently installed capabilities and compare to SRW simulations

⇒ take advantage of 'virtual' CHX beamline, that allows to easily match the 'real' setup in the simulations

CHX Commissioning: flux

-corrected magnetic field map of ID
-HDM with imperfections
-DCM with imperfections



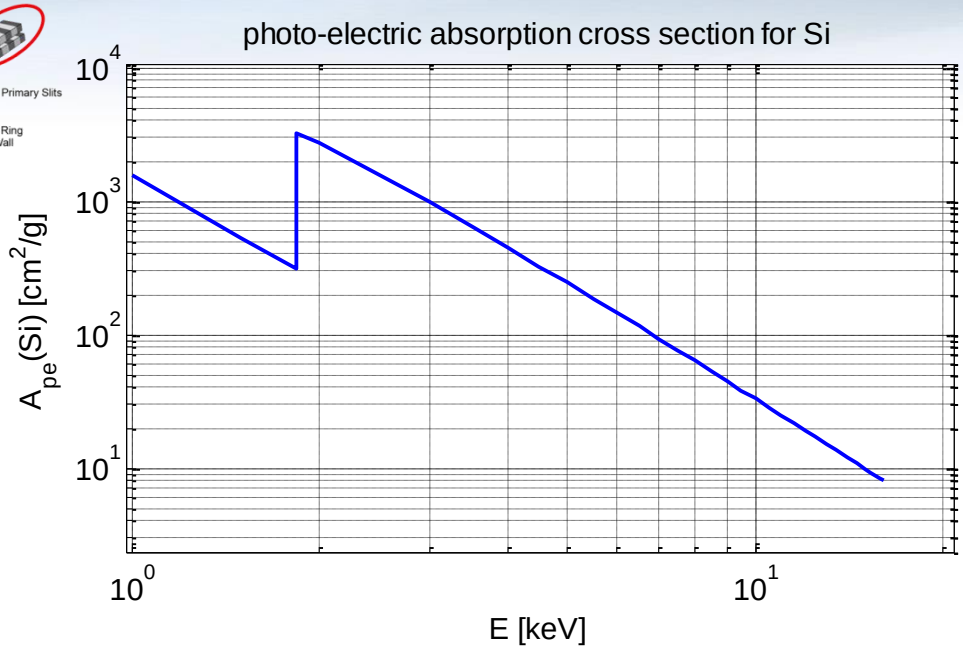


Photo-induced current I by X-ray flux ψ:

$$I = \psi e E[1 - \exp(-A_{pe} t_{Si} \rho_{Si})] / \varepsilon$$

e= 1.6022x10^{-19}C

L. Owen et al. J. Synchrotron Radiation (2009)

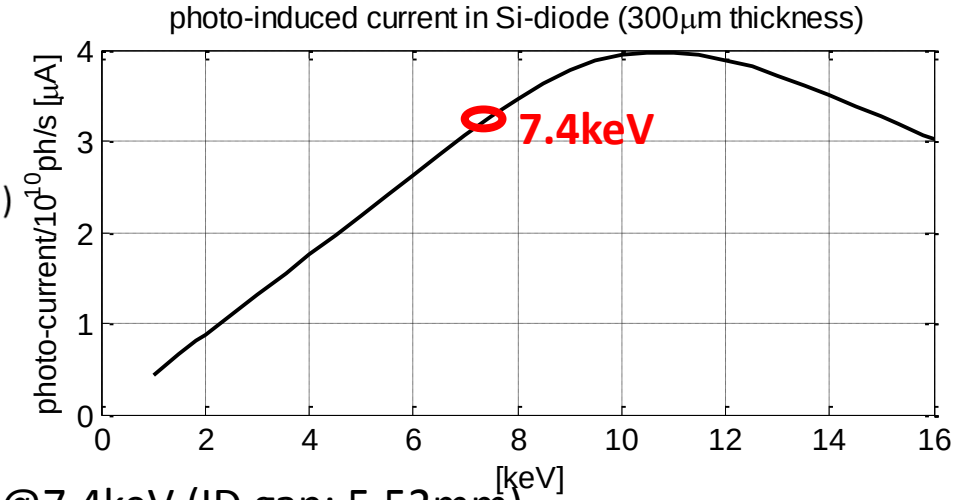
E: x-ray energy

A_{pe}: photoelectric cross section of silicon

t_{Si}=400um [0.04cm] (measured for S100VL by Owen et al.)

ρ_{Si}: density of Si [2.329g/cm^3]

ε: energy needed to create an electron-hole pair (3.66eV for Si)



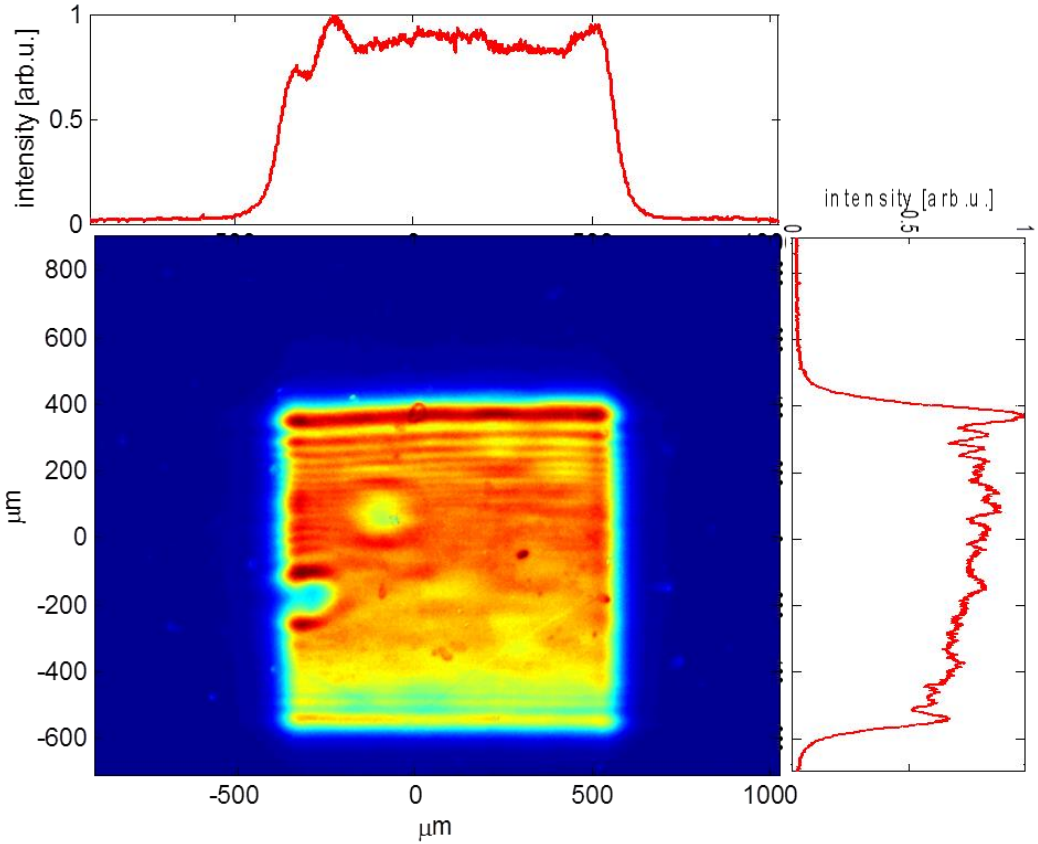
S2 (H x V) [mm^2]	photon flux /500mA [ph/s]	
	measured	simulated
0.1 x 0.1	6.3 x 10^{11}	6.4 x 10^{11}
0.2 x 0.2	2.0 x 10^{12}	2.6 x 10^{12}

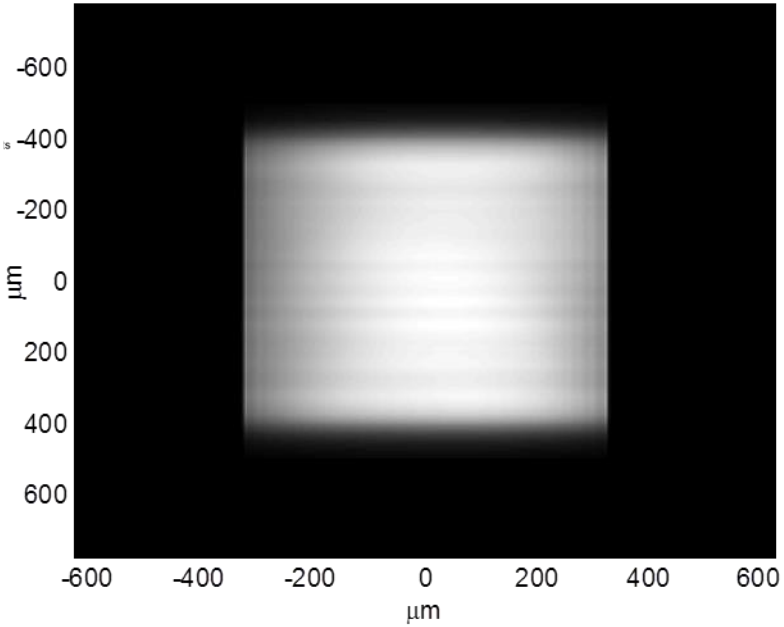
flux @7.4keV (ID gap: 5.52mm)

CHX Commissioning: unfocused beam

'design phase' unfocused beam, including metrology data of horizontal mirror:

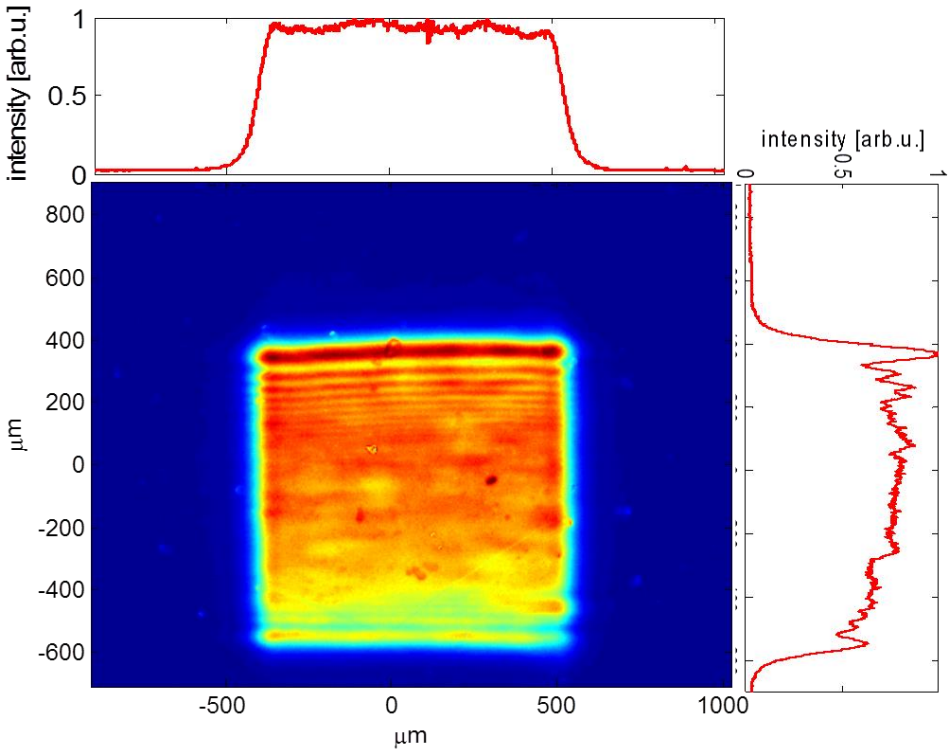
Reality check:



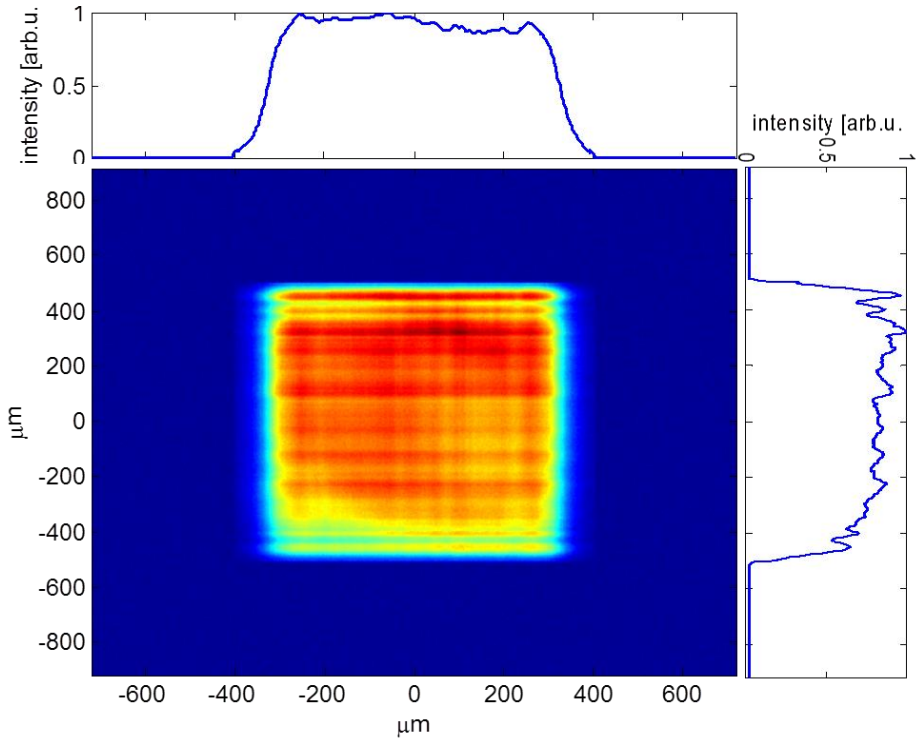


CHX Commissioning: unfocused beam

a better spot on the crystals:

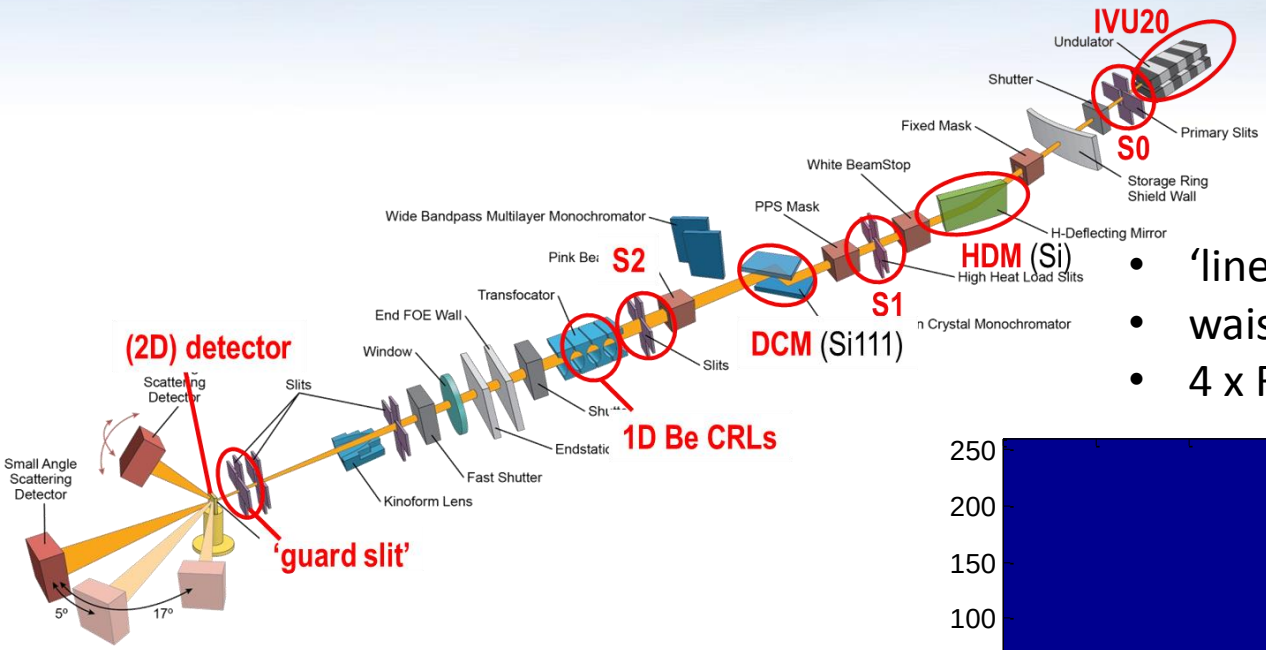


ME simulation with phase object for crystal imperfections (similar to HDM):

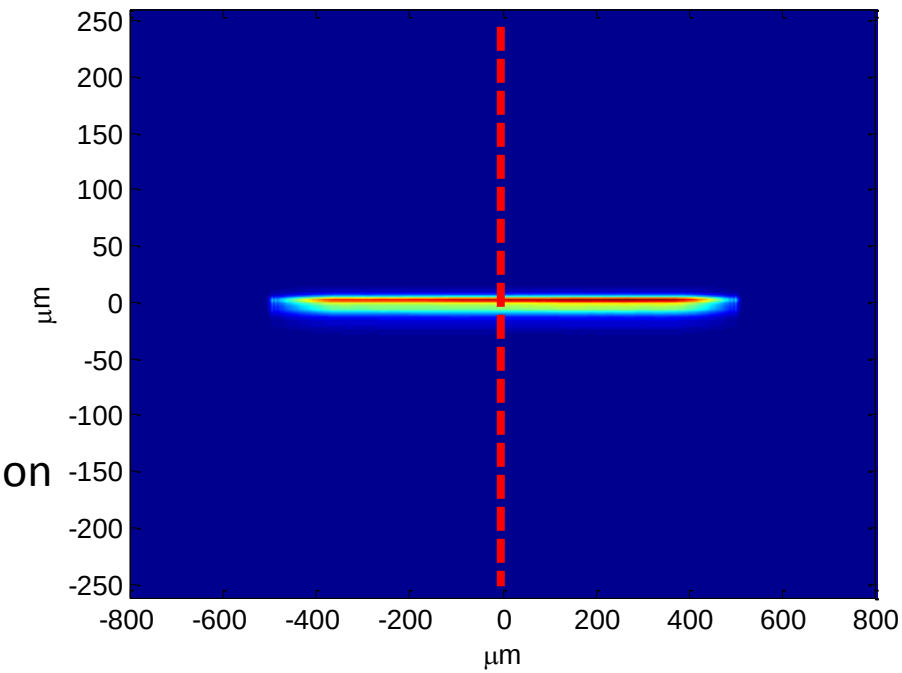


wish list: tool for solving the inverse problem for a phase object

Wavefront Propagation Simulations: vertical focus



- 'line focus' at 7416eV with Be CRLs
- waist before the sample position
- 4 x R=0.5 mm + 1x R=1.5 mm

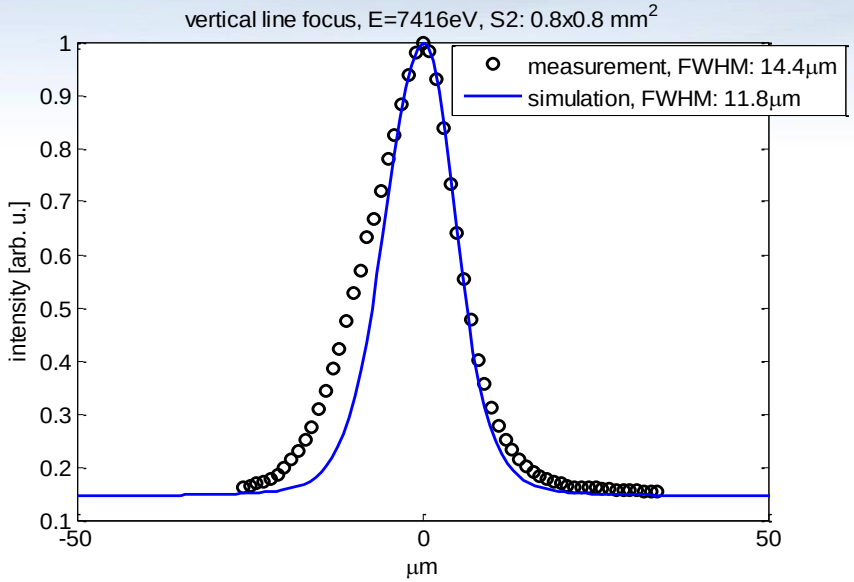


line focus measure with 'guard slit' scan

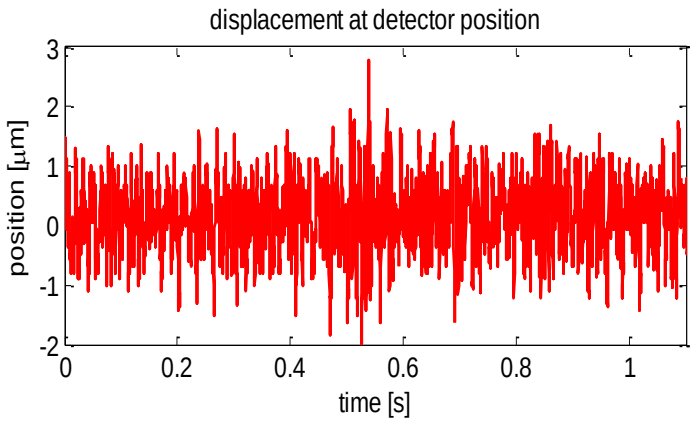
or

imaged with 2D detector at the sample position

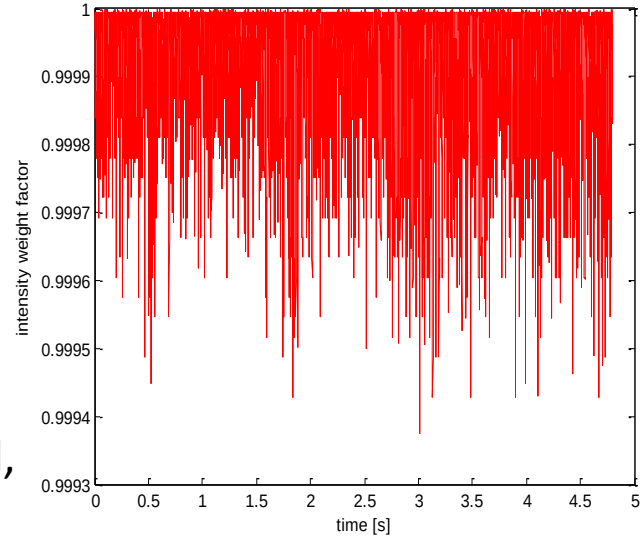
Wavefront Propagation Simulations: vertical focus

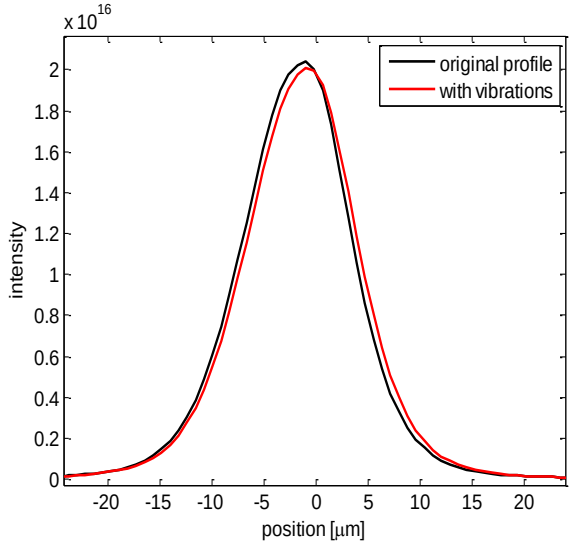


- convolution with resolution function for 1 μm slit gap
- data was collected without stabilizing feedback on 2nd DCM crystal, but vibrations are known from encoder readings -> add vibrations vibration of second crystal relative to the first) to the simulation data

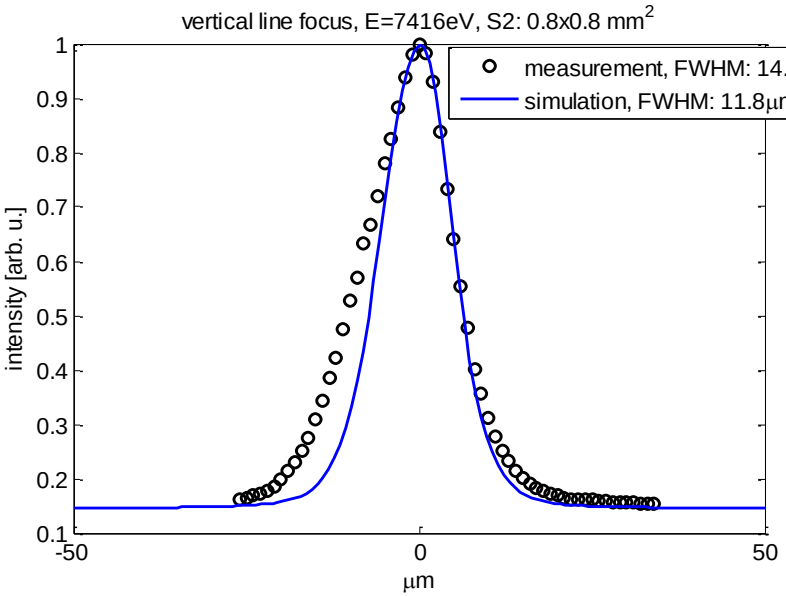


pitch vibrations of second crystal, recorded from encoder

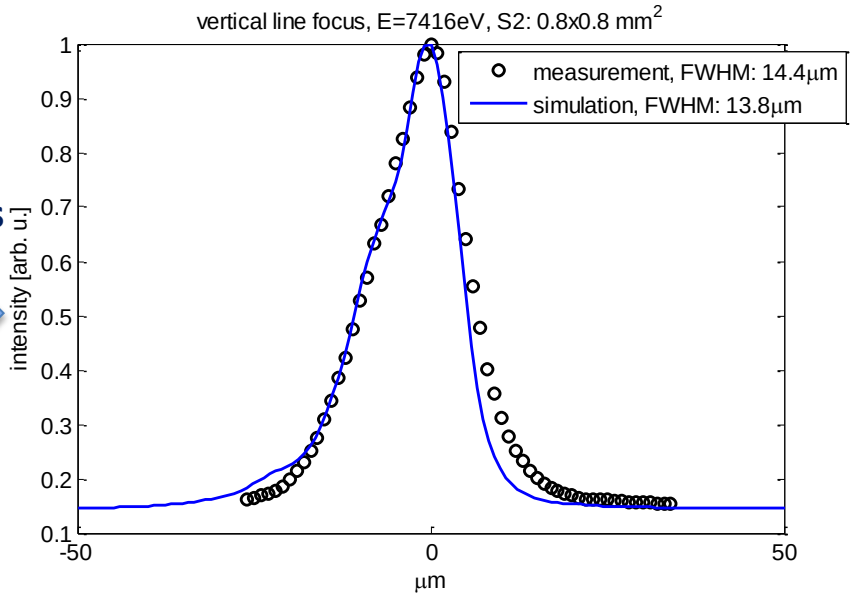




Wavefront Propagation Simulations: vertical focus



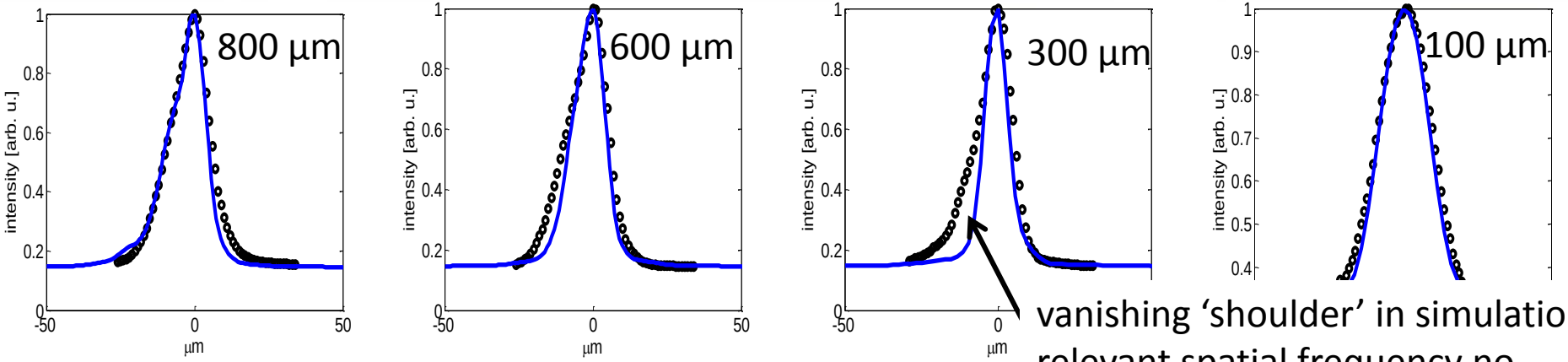
DCM imperfections



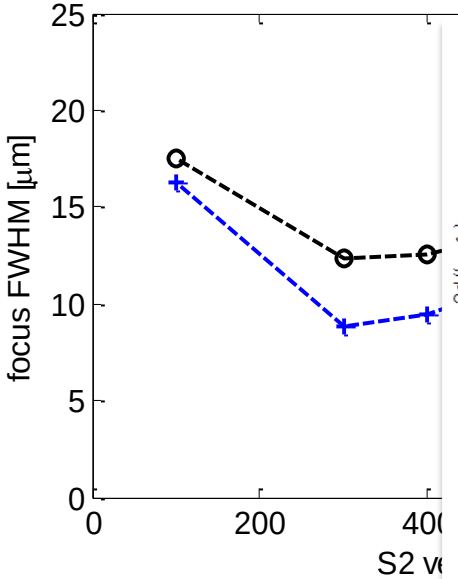
wish list: optical elements with vibrations (model and measured data)

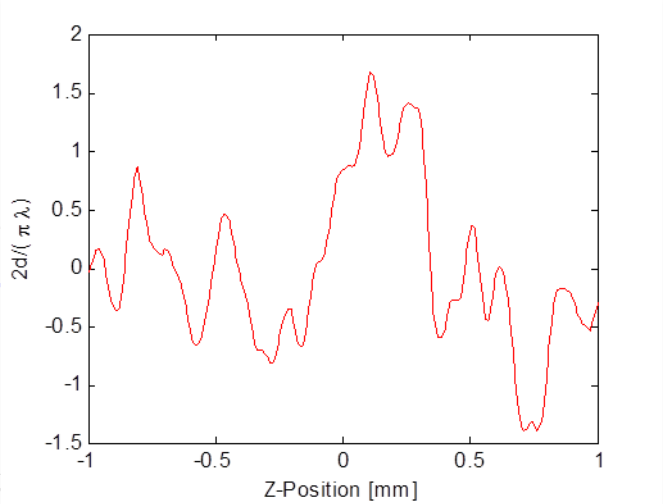
Wavefront Propagation Simulations: vertical focus

Closing S2 vertical gap:

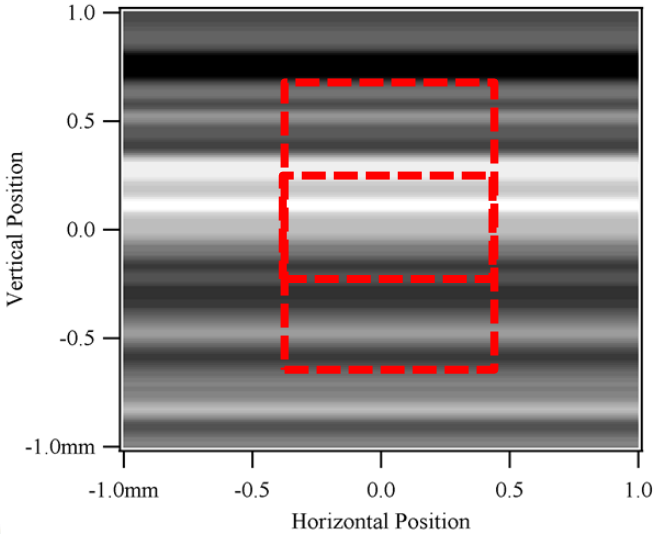


vanishing 'shoulder' in simulation: relevant spatial frequency no longer illuminated



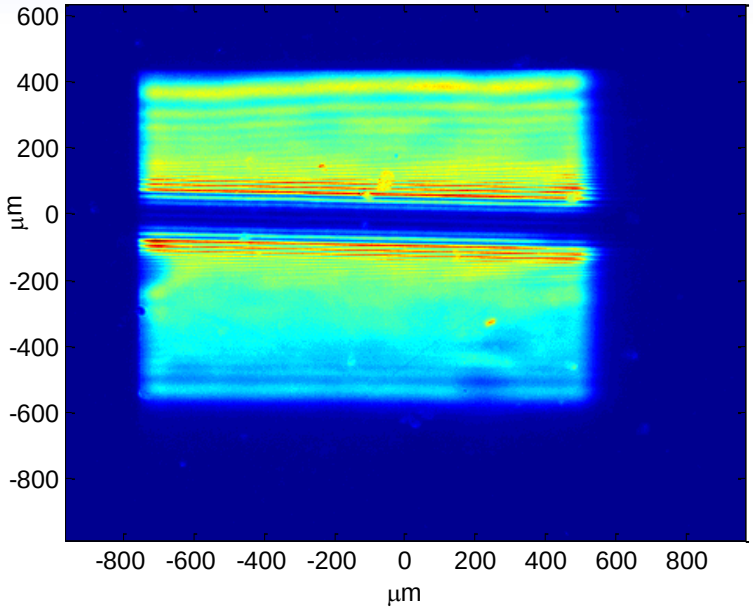


$rms_{DCM} \sim 20x\ rms_{HDM}$

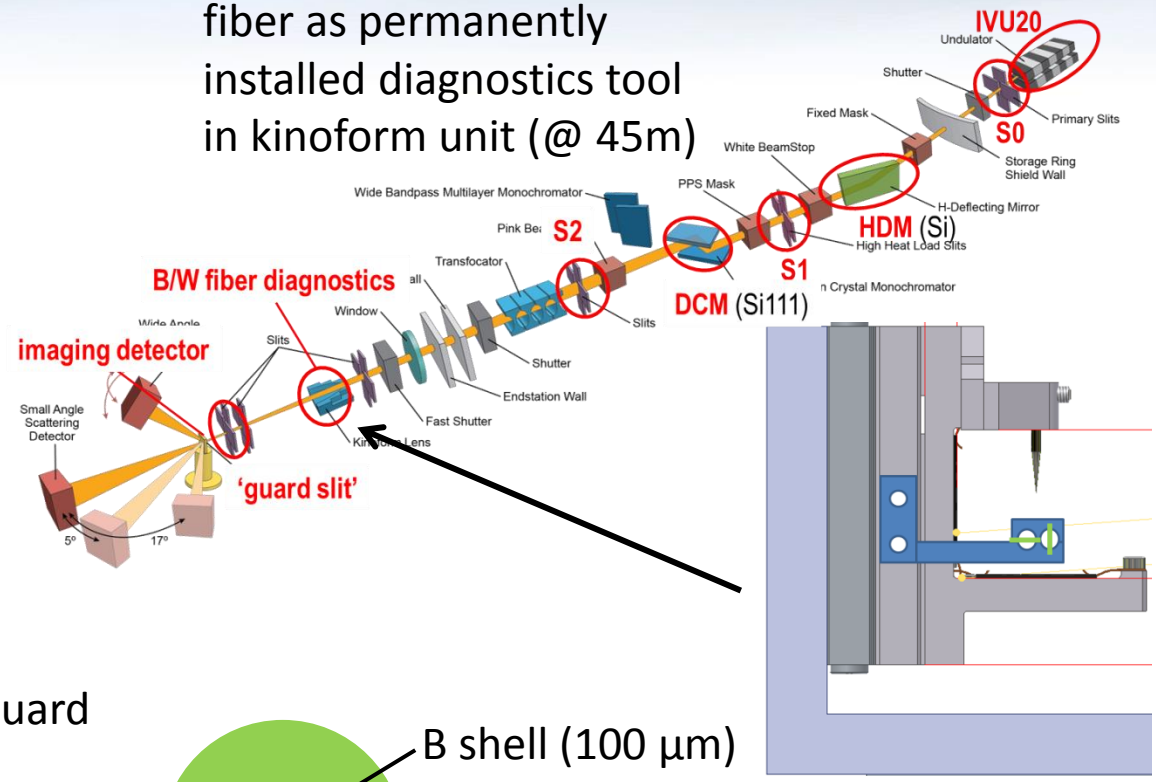


CHX Commissioning: coherent scattering from fiber

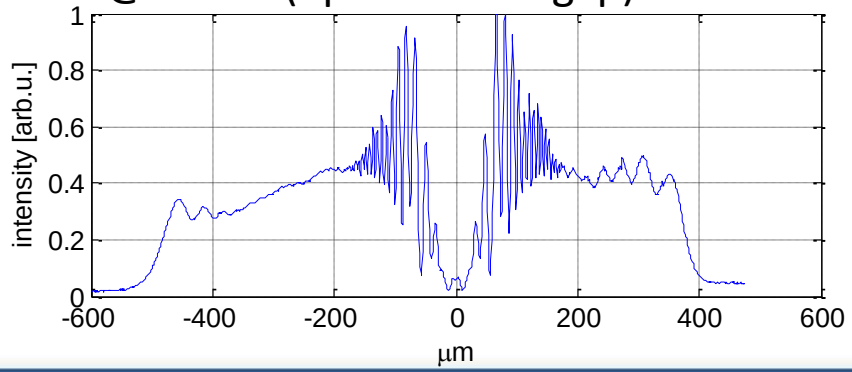
coherent scattering from fiber, measured with imaging detector @48.7m

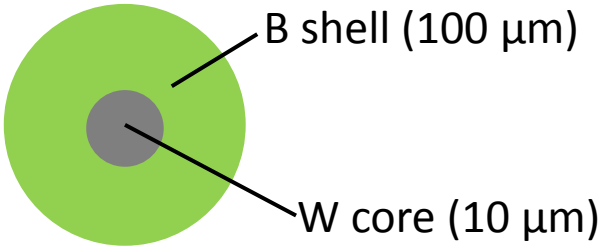


fiber as permanently installed diagnostics tool in kinoform unit (@ 45m)



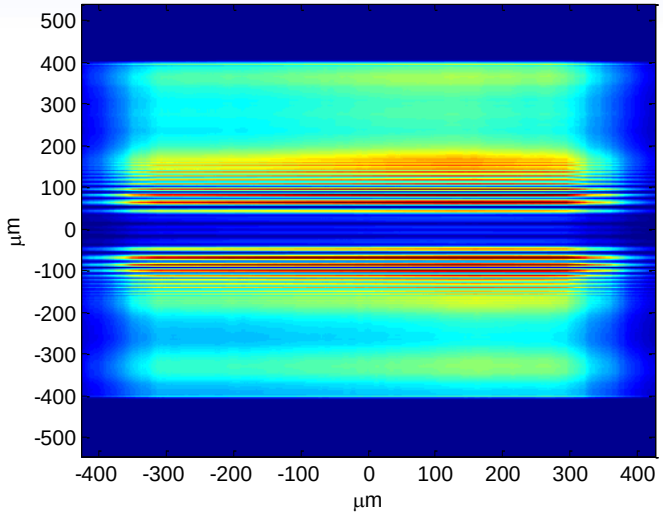
vertical cross-section, scanned with 'guard slit' @48.7m (1µm vertical gap)



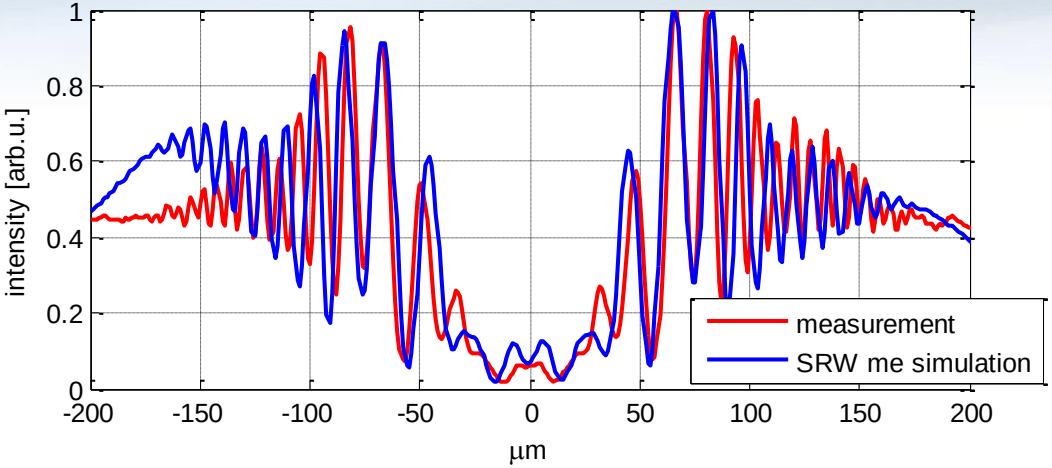


CHX Commissioning: coherent scattering from fiber

multi-electron wavefront propagation simulation of 2D scattering pattern



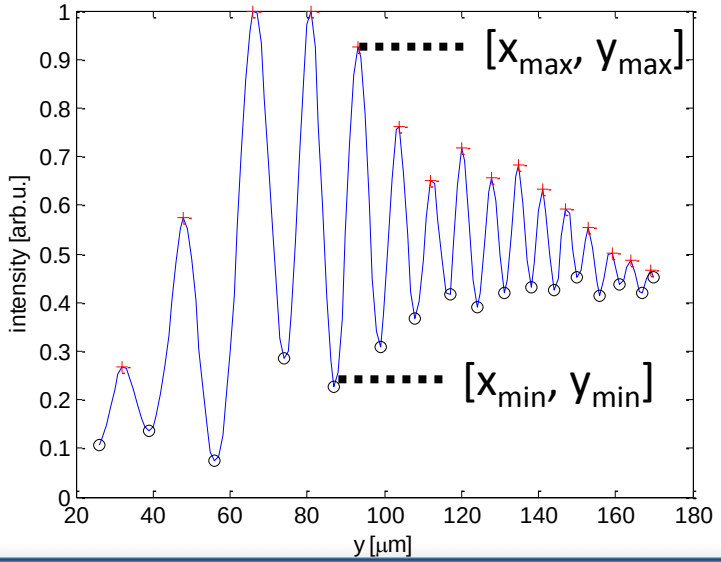
comprison of simulated and measured data: slit scan



qualitative, but not exact agreement: fiber not refined:

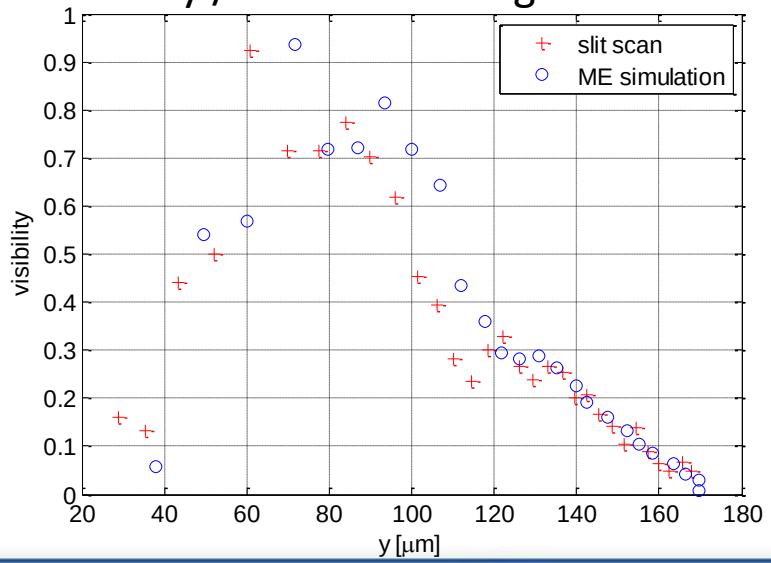
size / shape

electron density / interfacial roughness

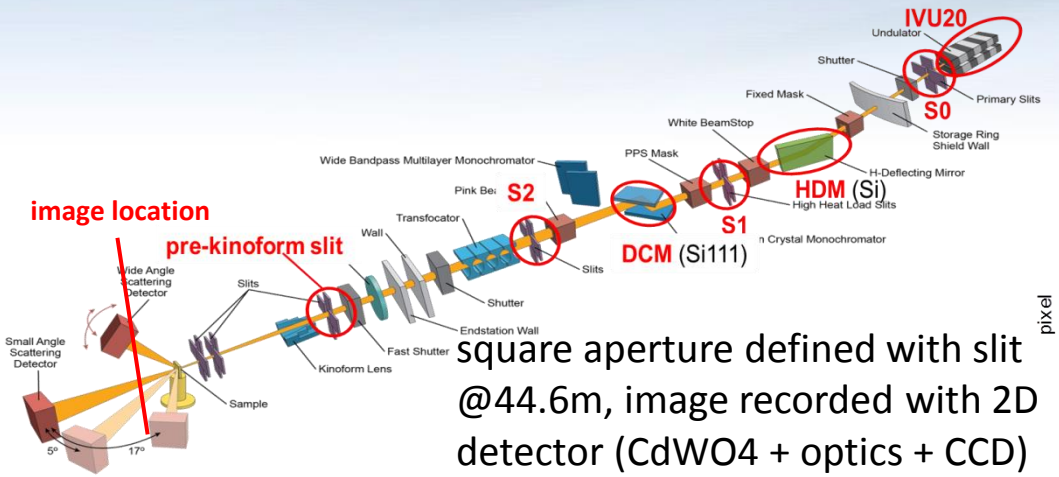


visibility=y_{max}-y_{min}

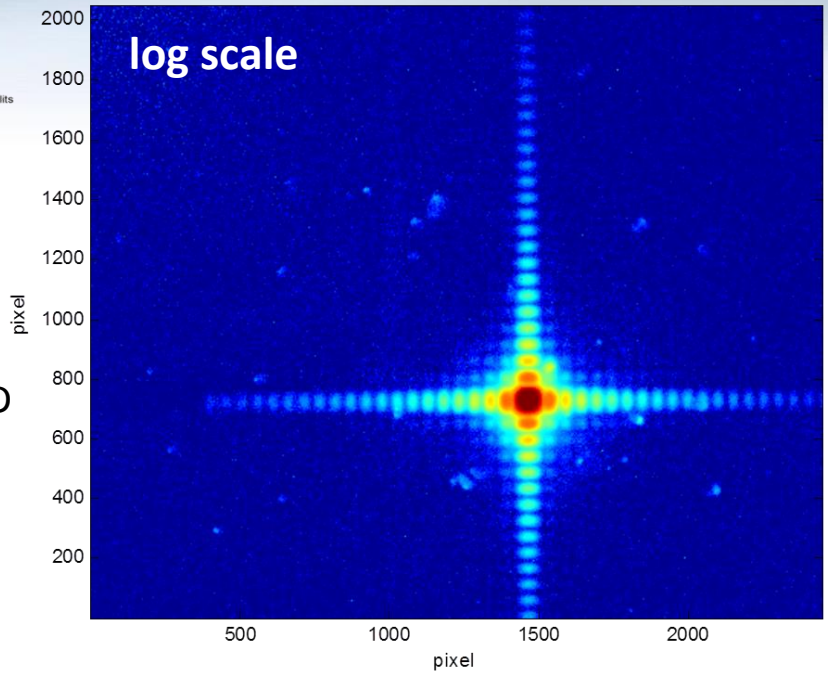
x= x_{max}-(x_{max}-x_{min})/2



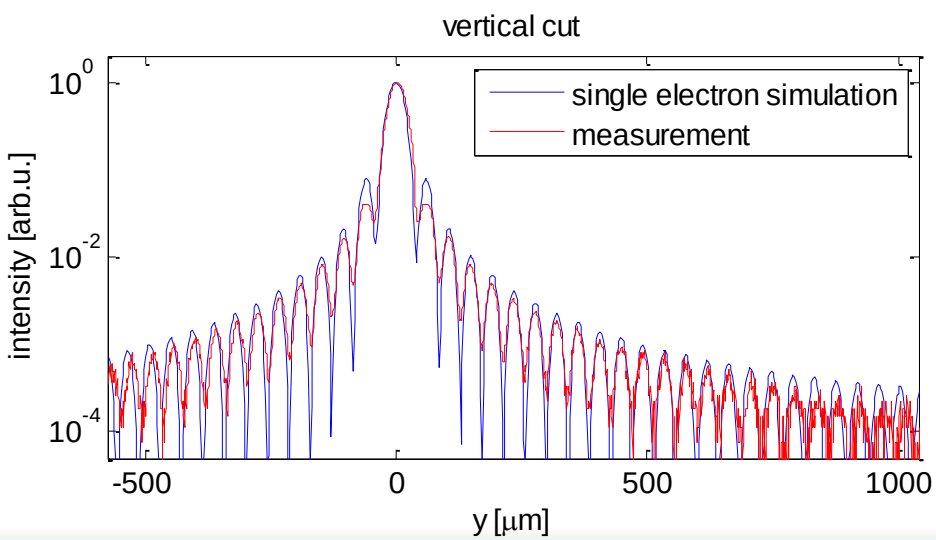
CHX Commissioning: coherent scattering from aperture

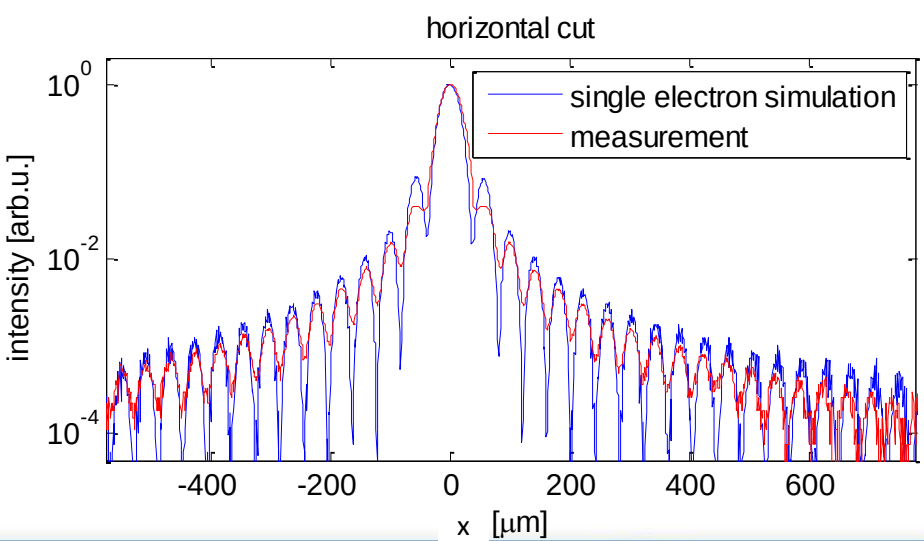


square aperture defined with slit @44.6m, image recorded with 2D detector (CdWO4 + optics + CCD) at the sample position (48.7m)



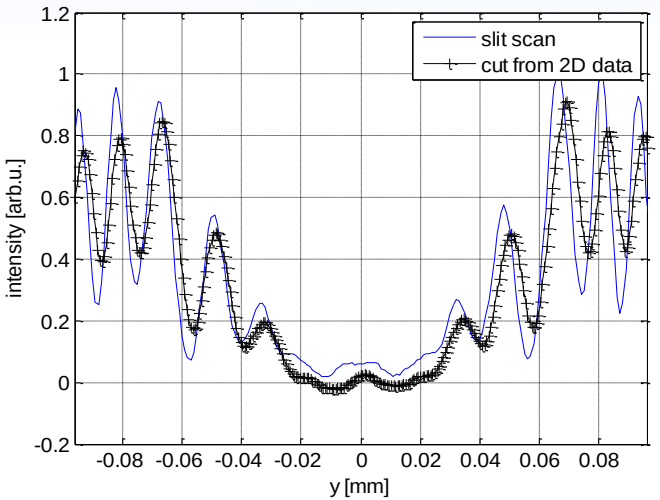
refinement of aperture dimensions using se emission: 19.4 x 18.5 µm² (h x v)





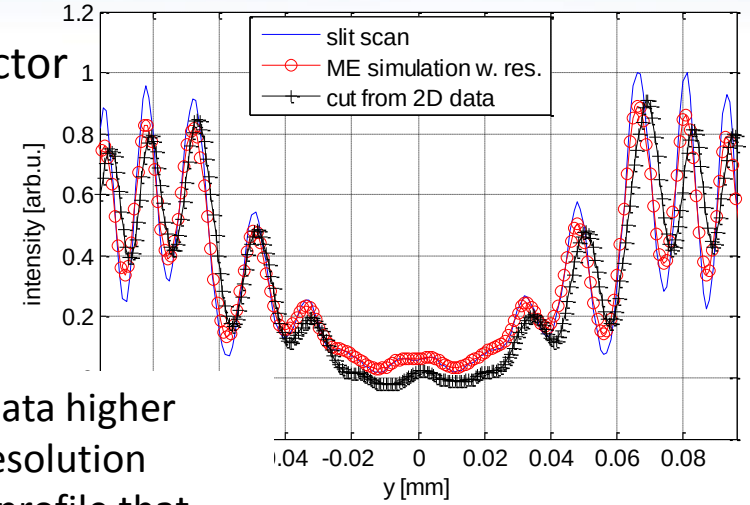
CHX Commissioning: coherent scattering from aperture

estimate of detector resolution from comparison of fiber data measured with slit scan and 2D detector



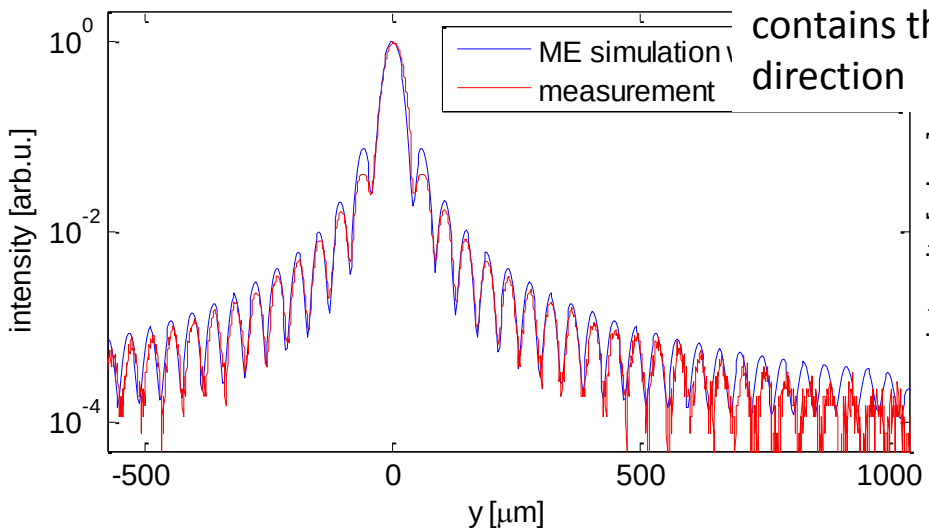
vertical cut

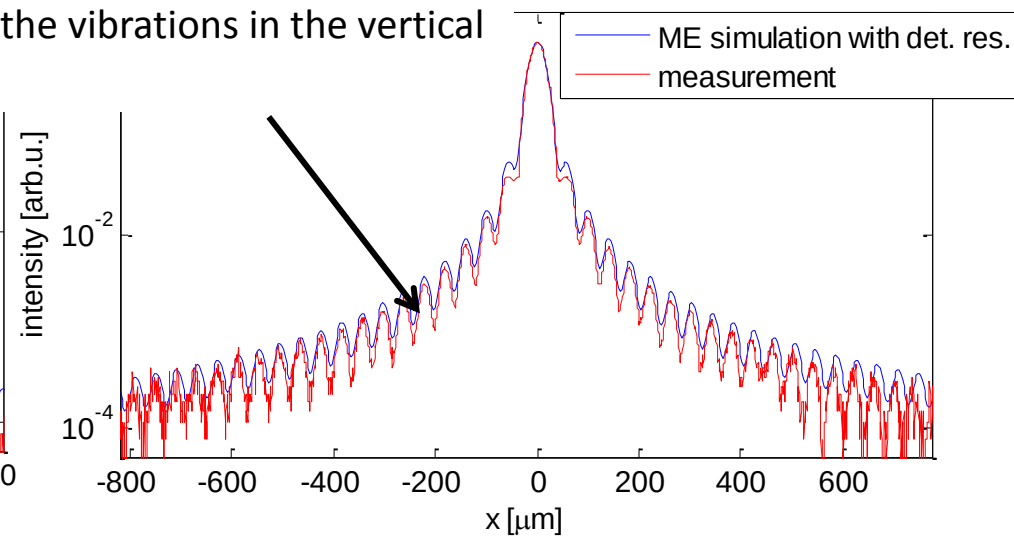
- nominal optical detector resolution: 2.4 µm
- Voigt profile



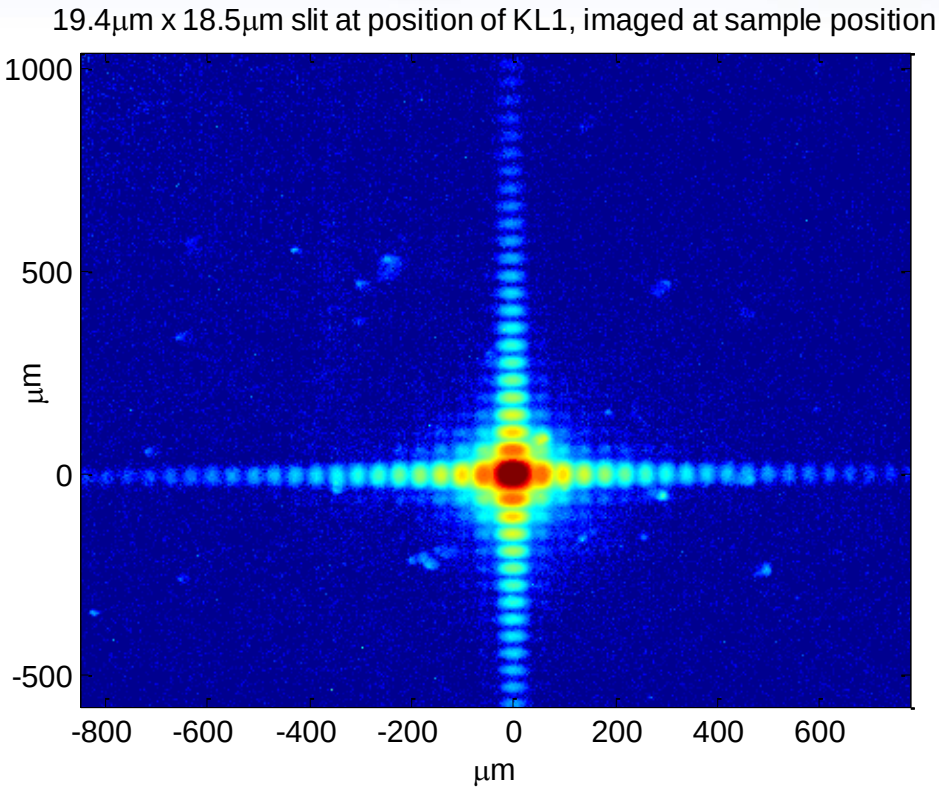
ontal cut

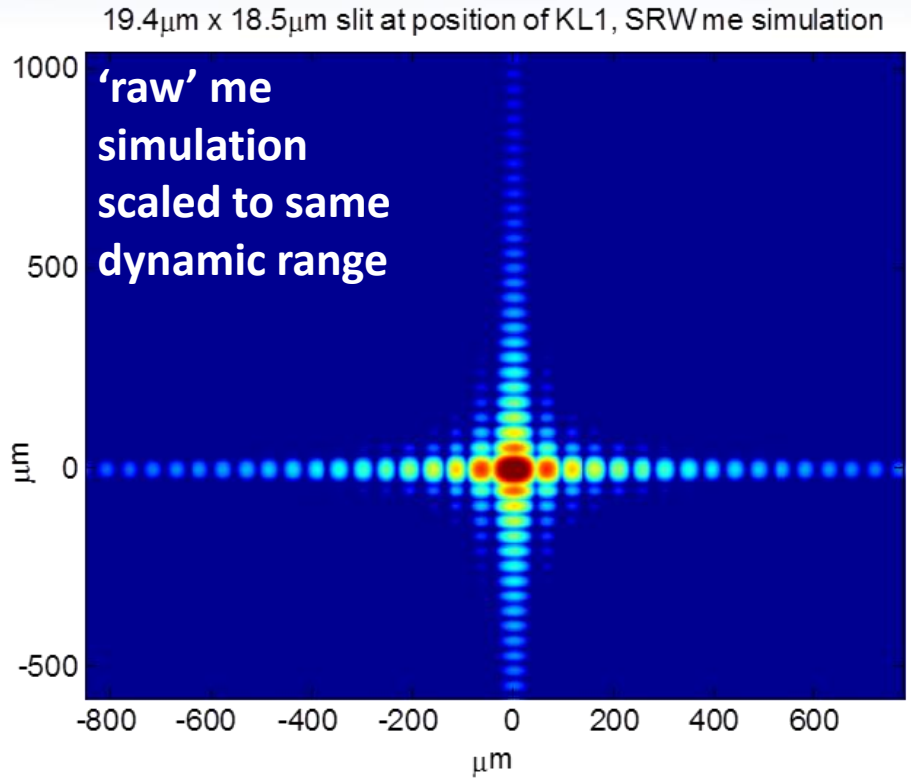
visibility in measured data higher than in simulation -> resolution determined with fiber profile that contains the vibrations in the vertical direction





CHX Commissioning: coherent scattering from aperture

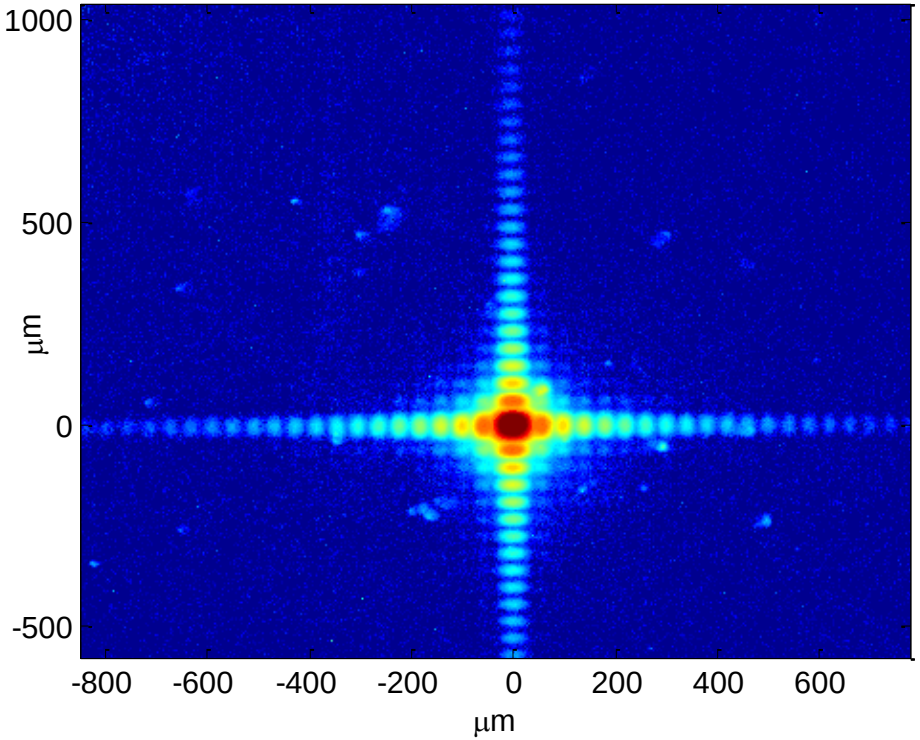




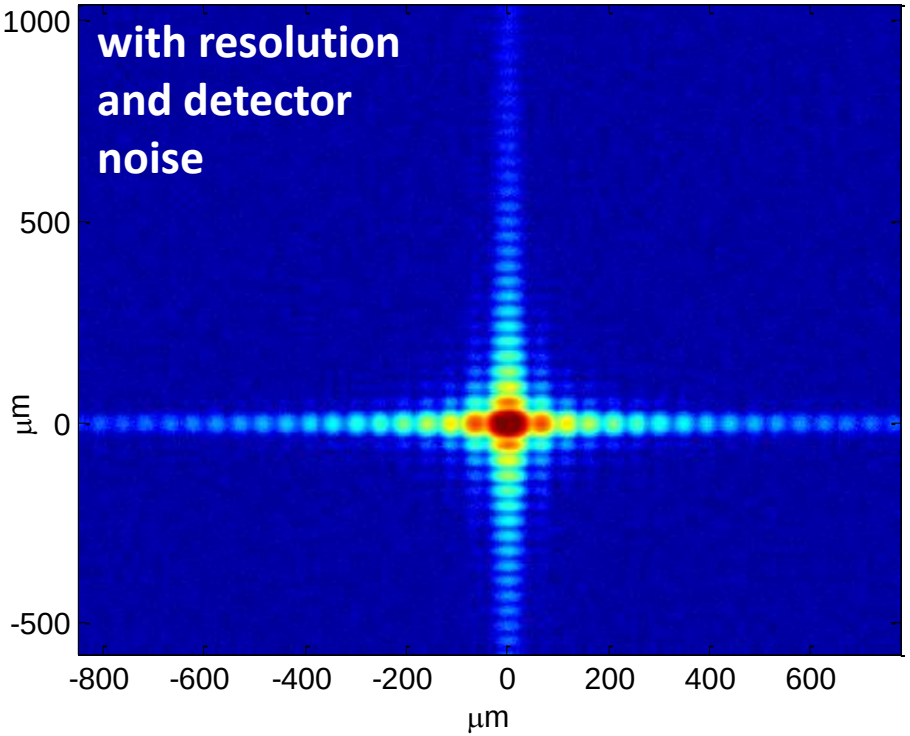
- reasonably good agreement between simulation and data
- only using measured parameters for convolution with detector resolution function
- measured performance consistent with imperfect DCM optics and ID magnetic field map

CHX Commissioning: coherent scattering from aperture

19.4μm x 18.5μm slit at position of KL1, imaged at sample position



19.4μm x 18.5μm slit at position of KL1, SRW me simulation

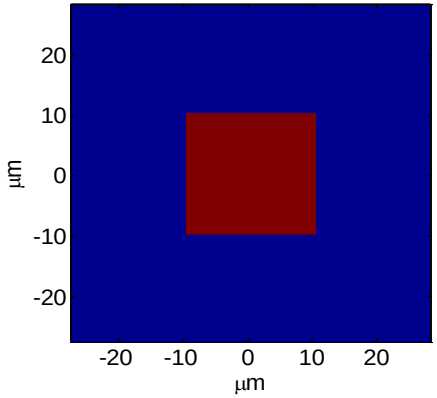


- reasonably good agreement between simulation and data
- only using measured parameters for convolution with detector resolution function
- measured performance consistent with imperfect DCM optics and ID magnetic field map

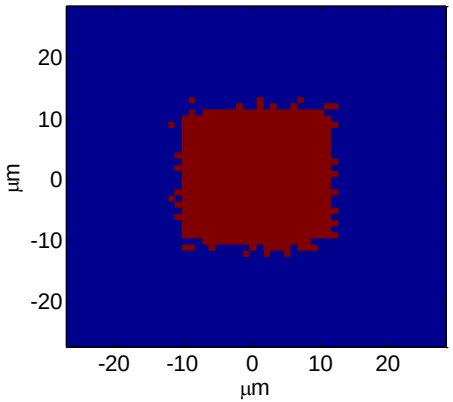
Wavefront Propagation Simulations

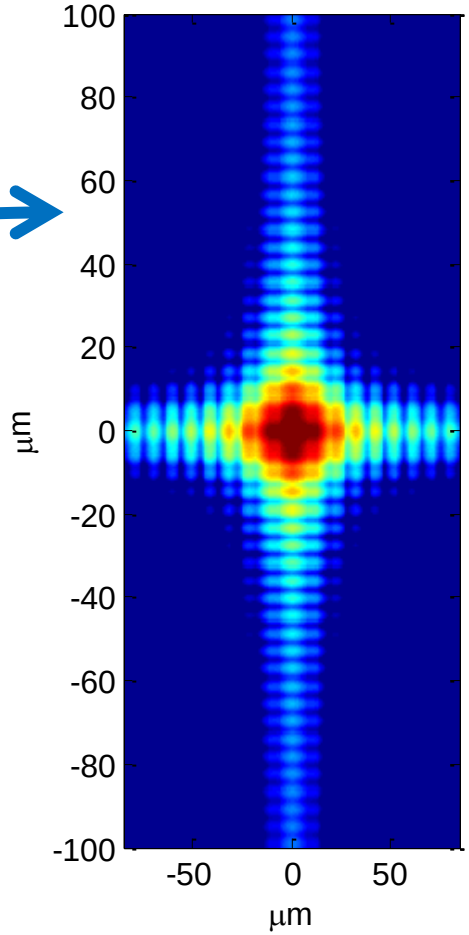
slits aren't perfect: (unfocussed) beam defined by knife edge square aperture at position of S3

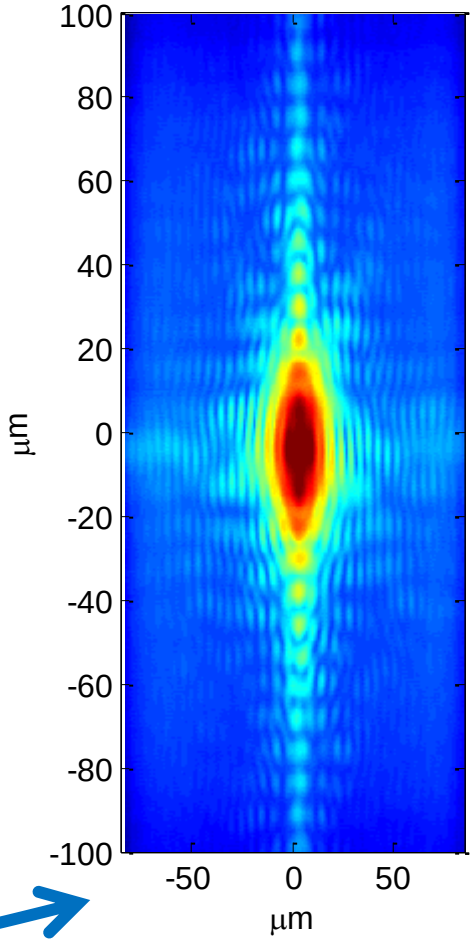
perfect knife edge



imperfect aperture

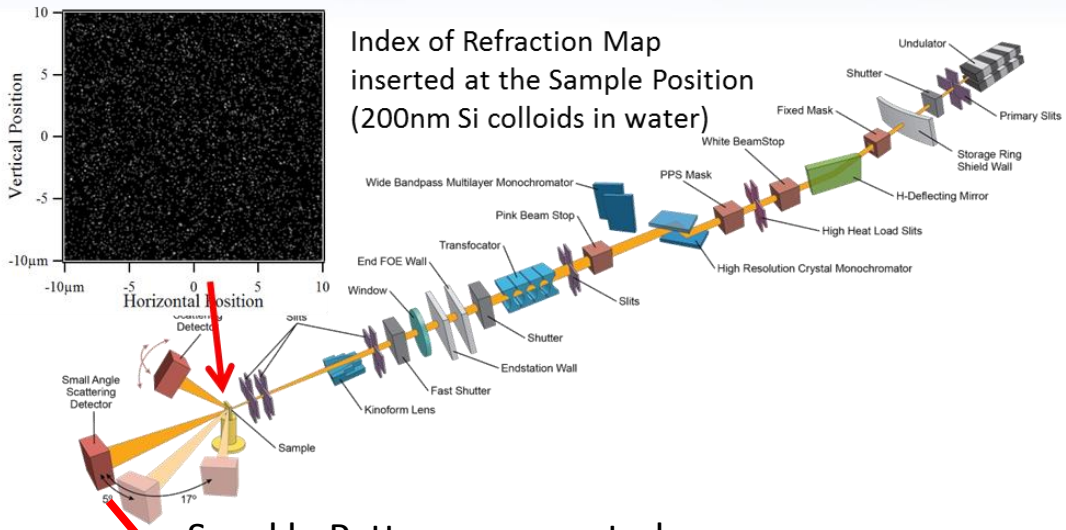




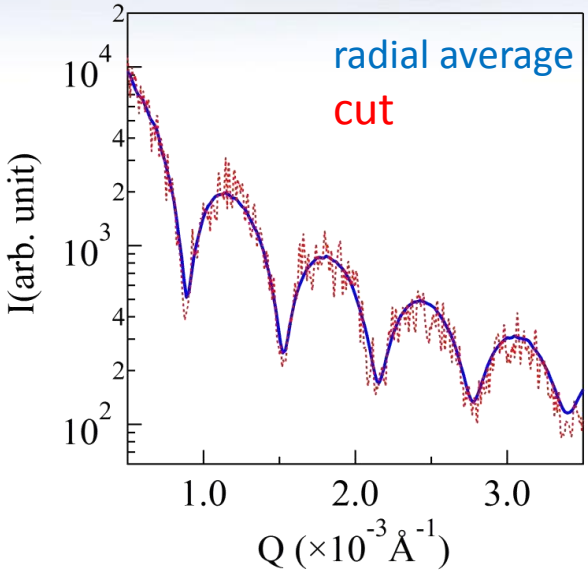


Wavefront Propagation Simulations: virtual experiments

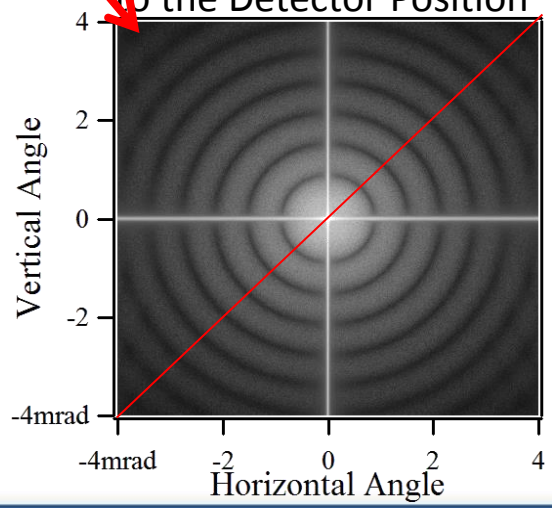
Known beamline performance and index of refraction maps for samples allow to simulate realistic scattering pattern for future experiments



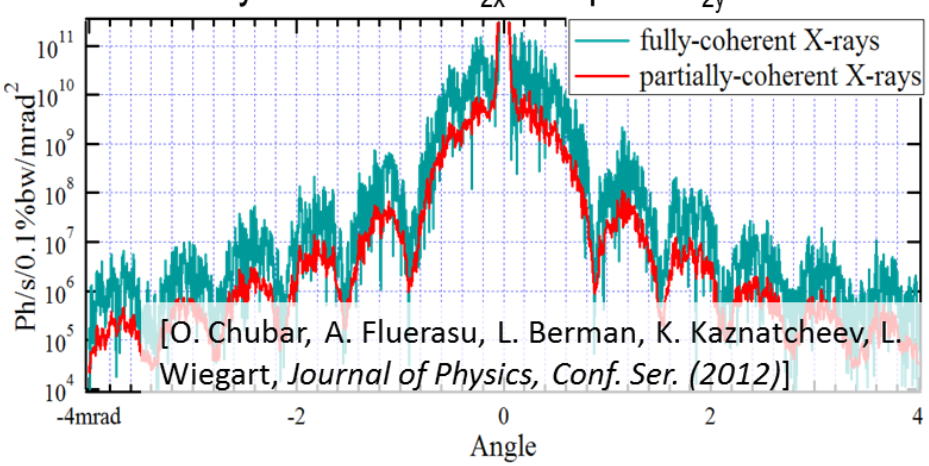
Index of Refraction Map inserted at the Sample Position (200nm Si colloids in water)



Speckle Pattern propagated to the Detector Position

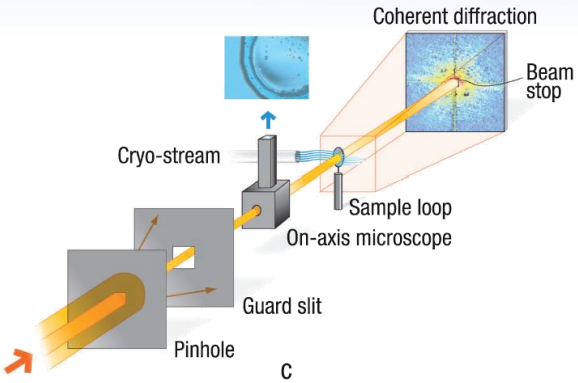


Partially coherent: ΔS_{2x}= 44 μm ΔS_{2y}= 1 mm

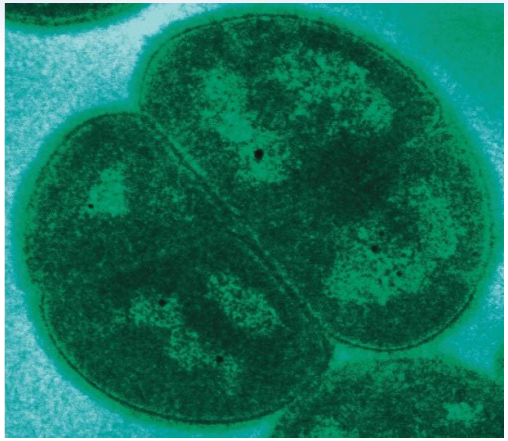


[O. Chubar, A. Fluerasu, L. Berman, K. Kaznatcheev, L. Wiegart, *Journal of Physics, Conf. Ser. (2012)*]

Wavefront Propagation Simulations: virtual experiments

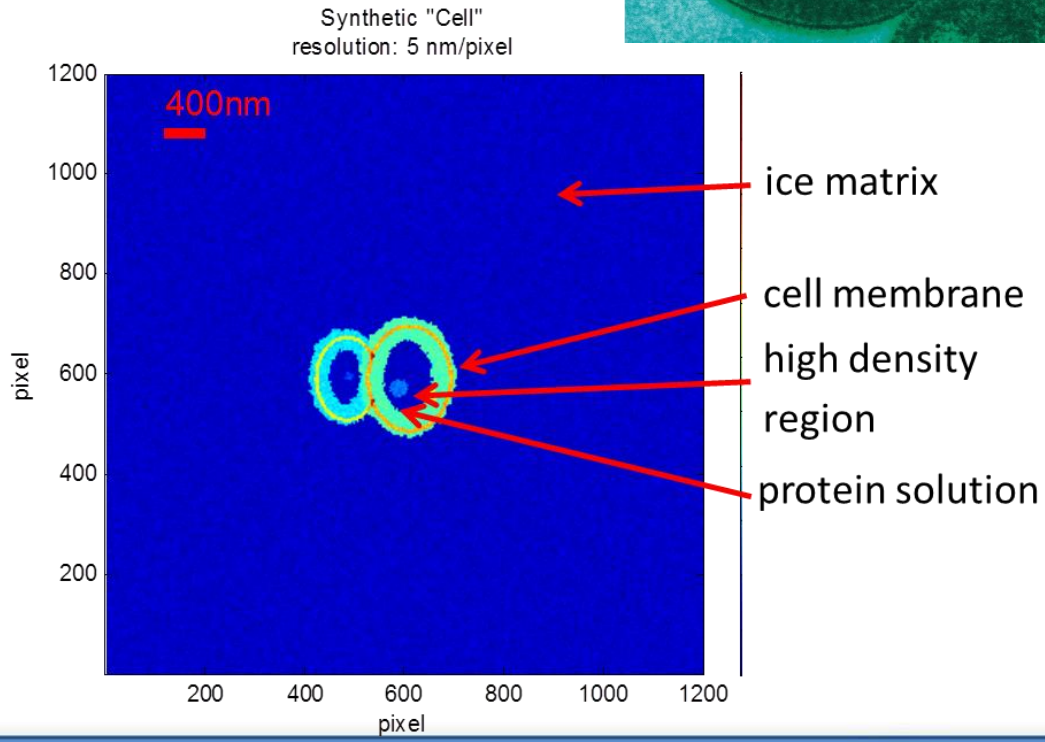


- example from CDXI: 'biological' sample with low electron density contrast
- full control over size and shape
- tunable phase object



	Composition	density+) [g/ccm]	σ [%]
ice matrix*)	H_20	0.94	2
cell membrane (70% lipid)	H62.5C3 1.5O6.3	1.0	10
hd region (80% protein)	H48.6C32 .9N8.9O8 .9S0.6	1.35	5
protein solution (70% protein)	H48.6C32 .9N8.9O8 .9S0.6	1.35	10

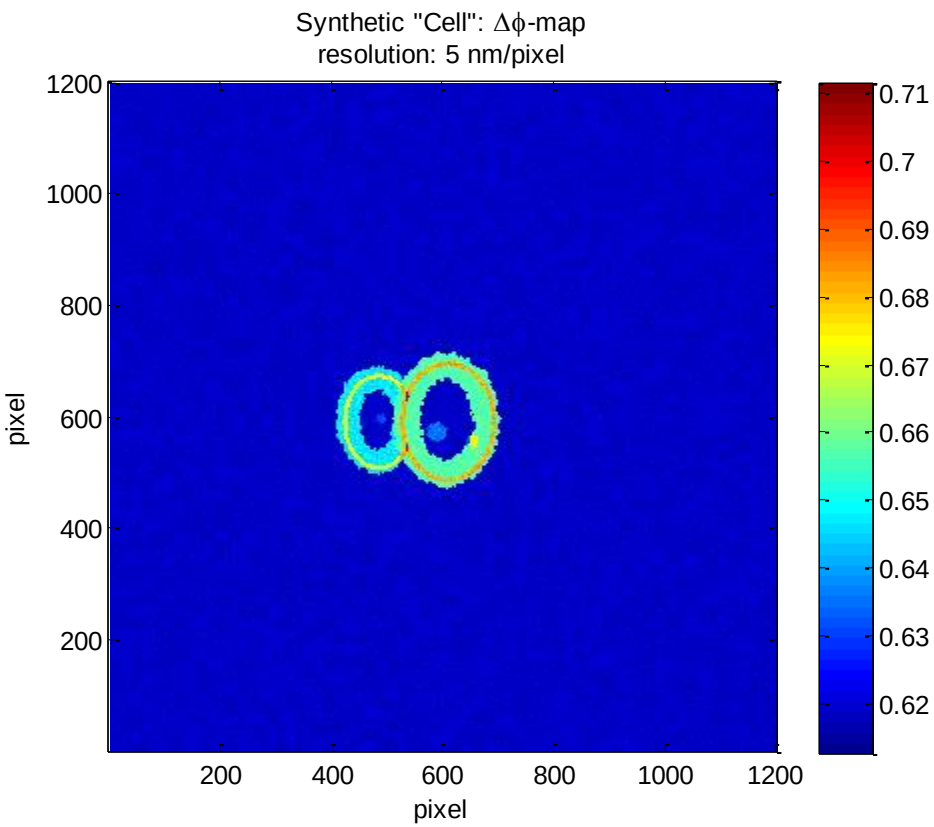
*) low density amorphous ice
+) density of non-diluted component

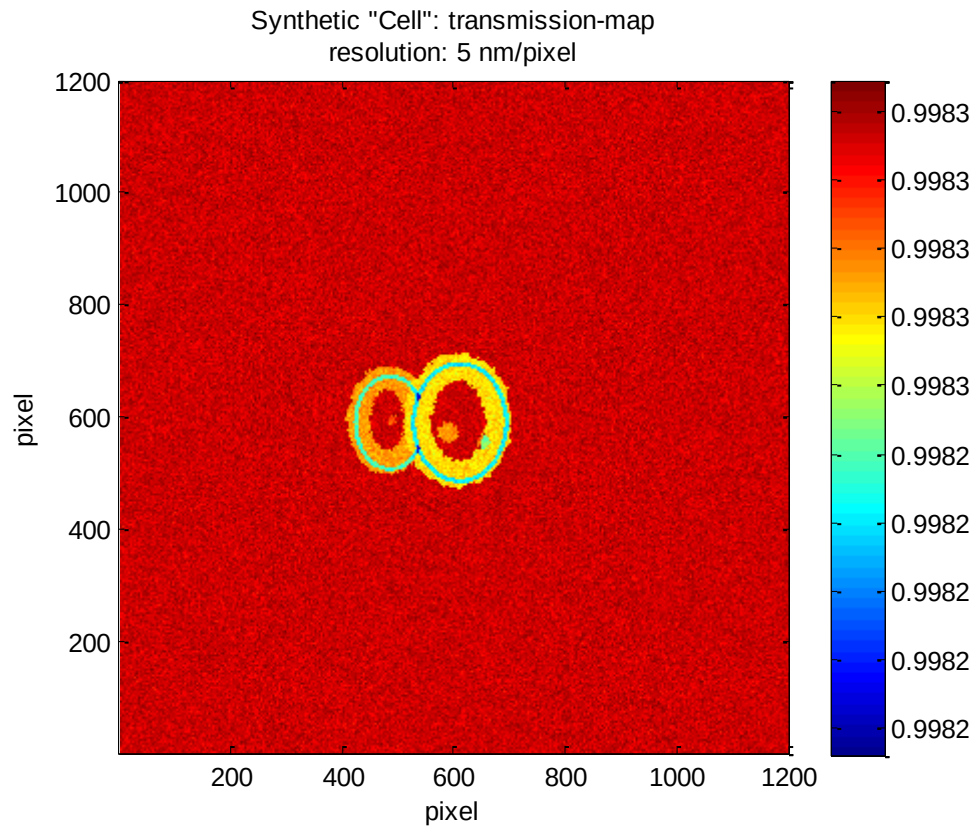


Wavefront Propagation Simulations: virtual experiments

Phase shift: $\Delta\Phi = \frac{2\pi}{\lambda}\delta d$

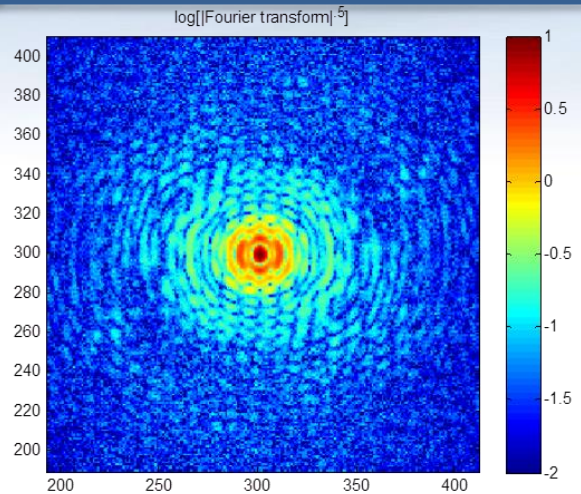
Transmission: $T = e^{-\mu d}$ $\mu = \frac{2\pi}{\lambda}\beta$



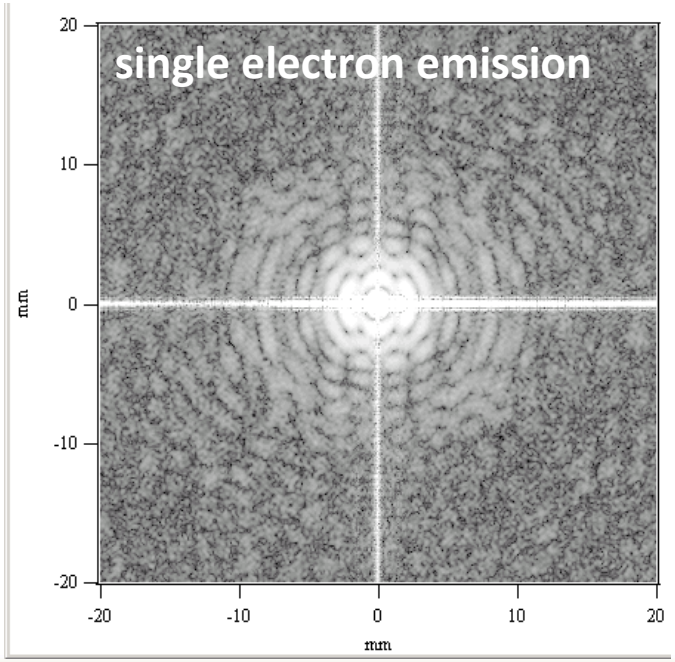


Wavefront Propagation Simulations: virtual experiments

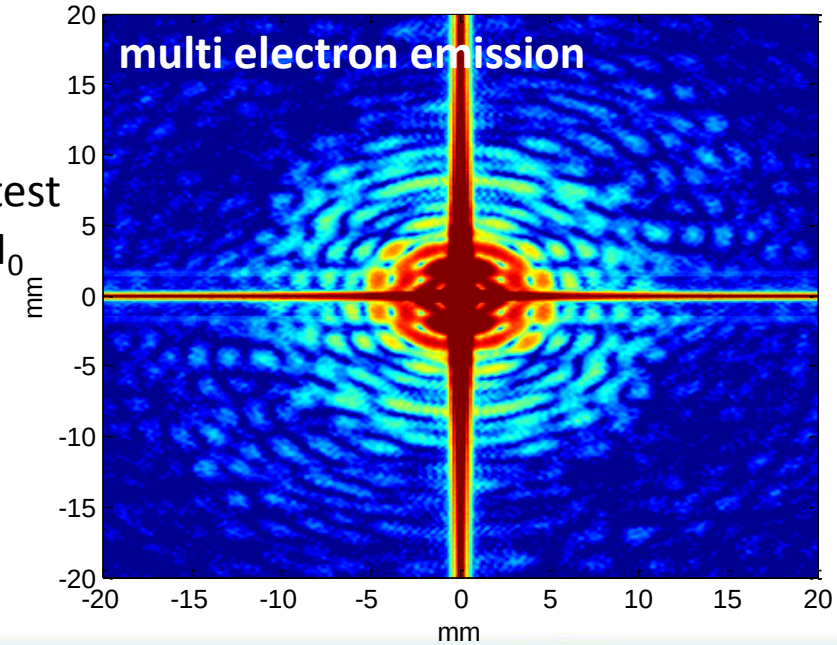
Direct FFT of the 'sample'



'Sample' in beamline, propagated to detector 10m downstream from sample



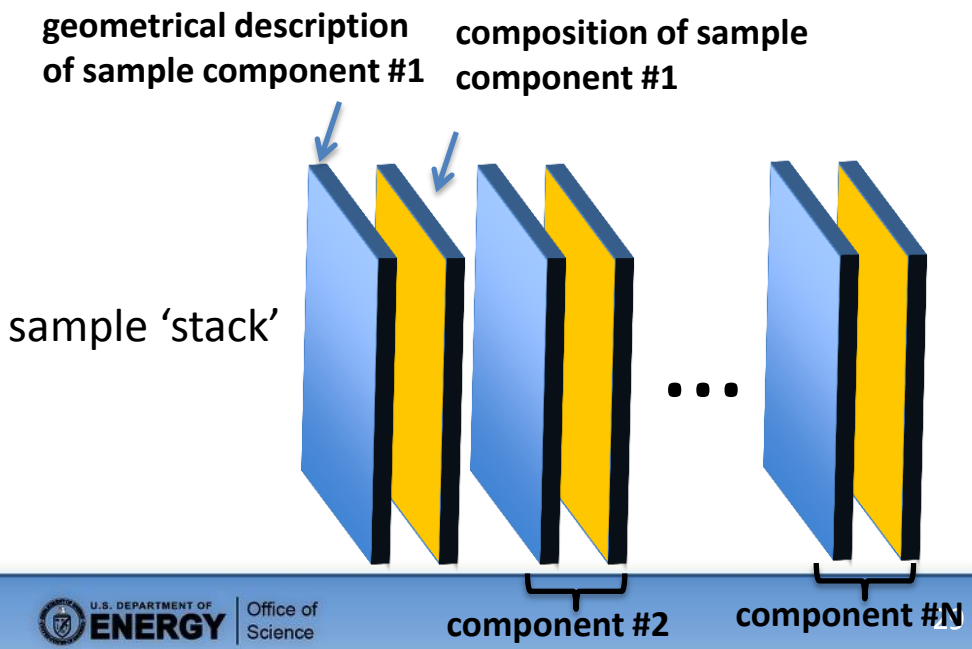
intensity of brightest speckles is ~$10^{-8}*I_0$



Wavefront Propagation Simulations: virtual experiments

wish list: unified, more flexible description of ‘virtual’ samples

- approach so far: calculate transmission and phase shift maps from sample’s geometry and complex index of refraction
  -> need to ‘prepare’ new sample when changing energy
  -> cannot ‘prepare’ identical sample for different energy, if randomness is involved…
- proposal for alternative description: stack of sample ‘geometries’ and composition:



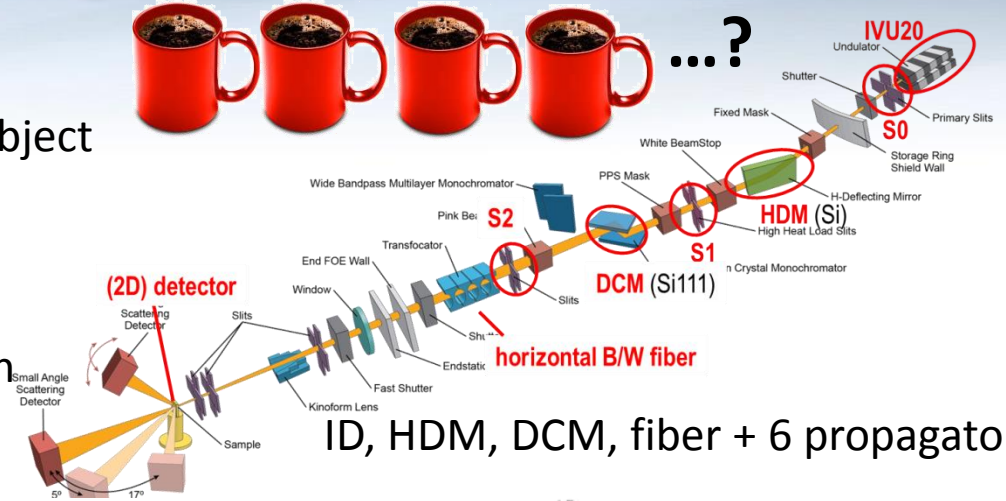
- energy dependent complex index of refraction from database
- total sample phase and transmission maps from sum over the stack

Wavefront Propagation Simulations

How long does a simulation take?

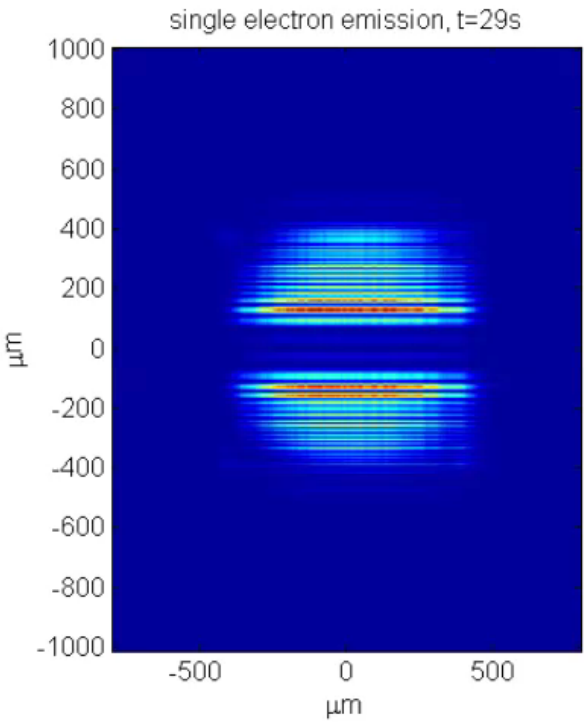
...?

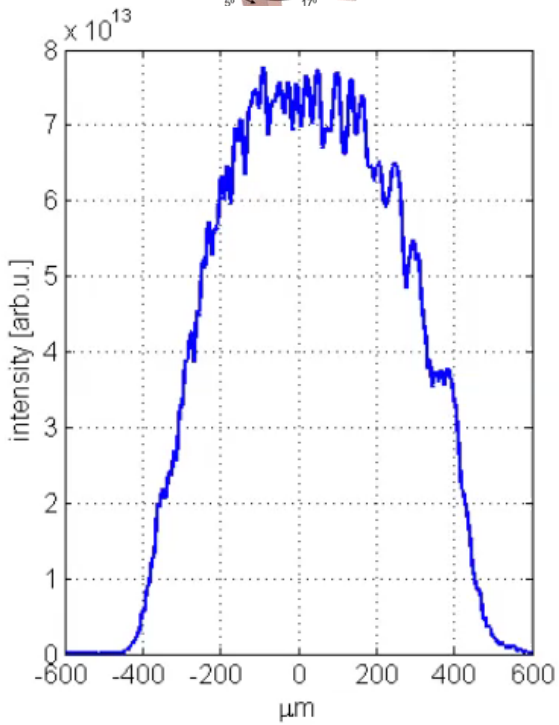
- number of optical elements / phase object
- number of propagators
- wavefront size / sampling
- ....
- number of cores used for computation

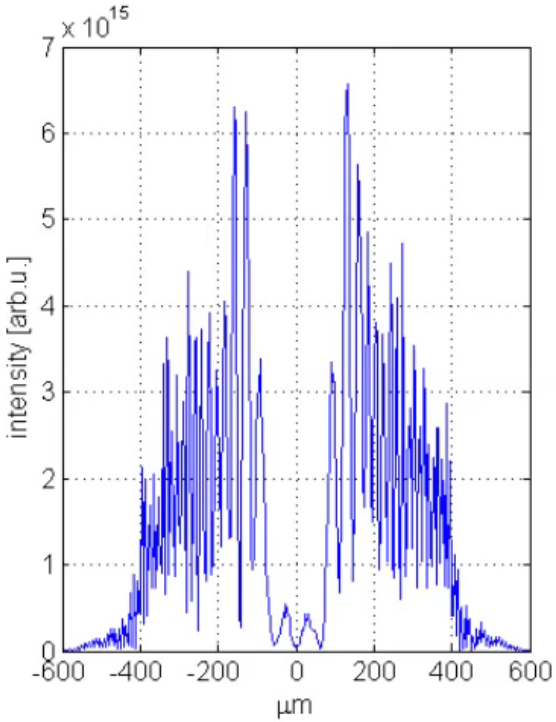


ID, HDM, DCM, fiber + 6 propagators

me-simulation: using 6 cores on a server







Wavefront Propagation Simulations

How long does a simulation take?

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- ....
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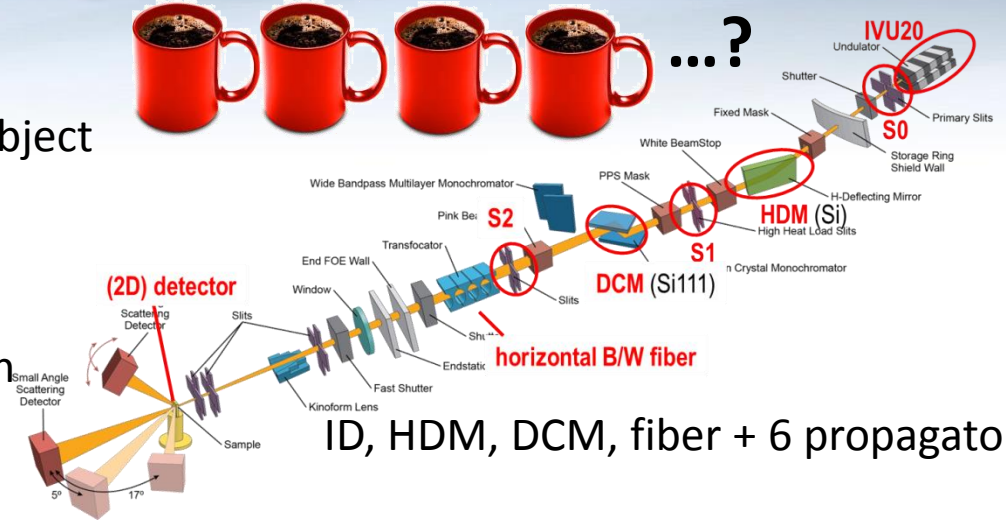
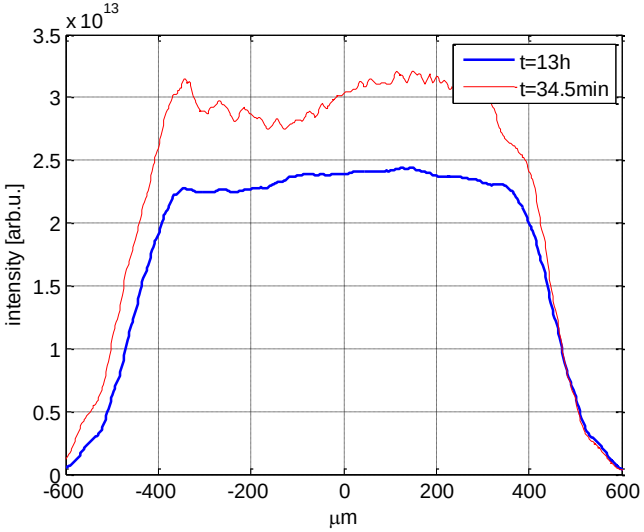
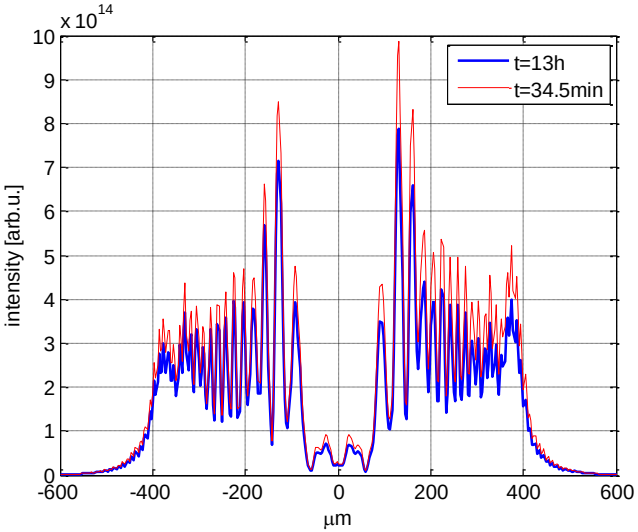


ID, HDM, DCM, fiber + 6 propagators

me-simulation: using 6 cores on a server





reasonably close after ½ h
parallel problem: scales with number of nodes, e.g. 30 cores -> ~6 min, etc.

parameters **NOT** optimized for speed

Summary

- Performance of the CHX beamline so far as expected, taking into account the quality of DCM crystals and small vibrations arising from missing feedback-loop

- the ‘virtual CHX beamline’ implemented in SRW has proven to be versatile, quickly to adapt to match settings of the real CHX beamline

- Simulations are robust, i.e. do not require tweaking of propagation parameters (wave front size, sampling,…) over a large range of operating parameters of the CHX beamline

- development of a ‘virtual’ CHX beamline with user friendly parameter input underway

- Simulations will help in the future to not only check and optimize beamline performance, but will become a tool for the design of experiments and data interpretation

First Users of the CHX 'virtual beamline'

- required simulation of beam propagation through CHX beamline for design optimization of lithographic samples for user beamtime in October
- 'virtual samples' created, simulation pending

beam focusing/divergence
E=9578eV

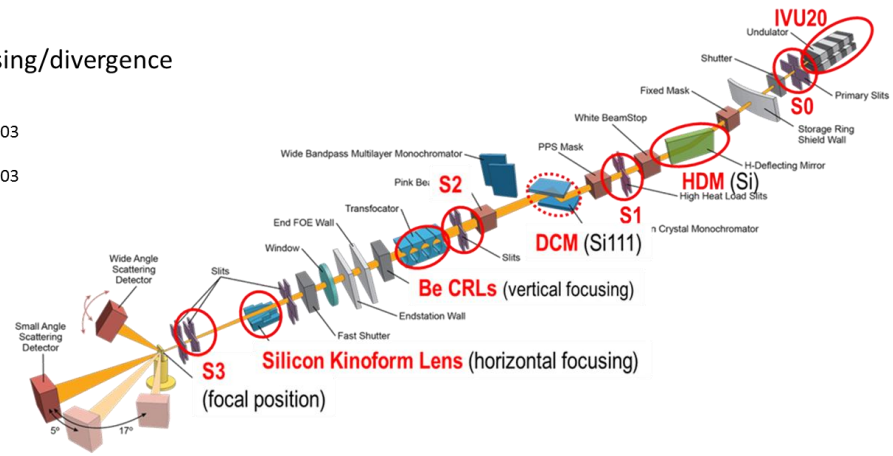
rminCRL1 = 0.5e-03
nCRL1 = 7
rminCRL2 = 1.5e-03
nCRL2 = 1
CRL_dz = 0.25

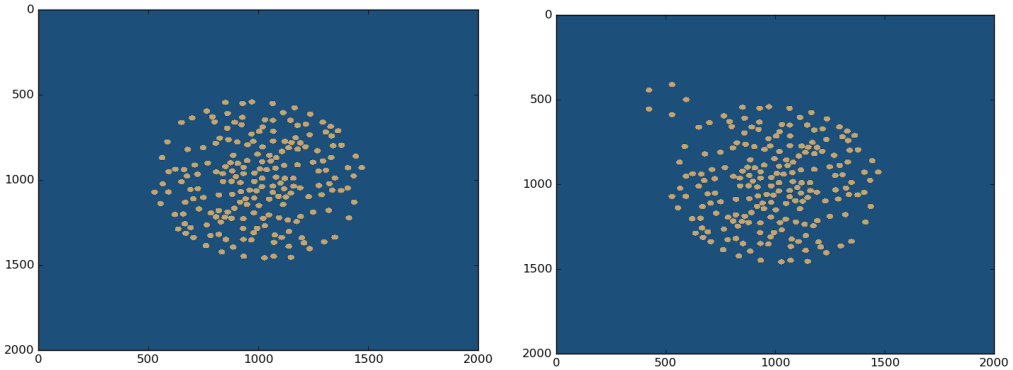
#primary slit:
dxS0 = .8e-3
dyS0 = 1.2e-3

#pink beam slits:
dxS1 = .8e-3
dyS1 = 1.0e-3

#S2:
dxS2 = .05e-03
dyS2 = .8e-03

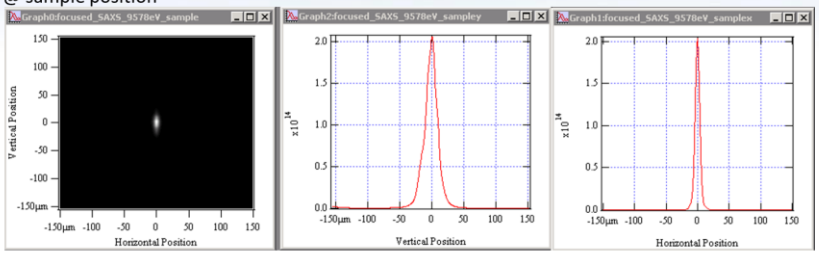
#S3:
dxS3 = .05e-03
dyS3 = .05e-03



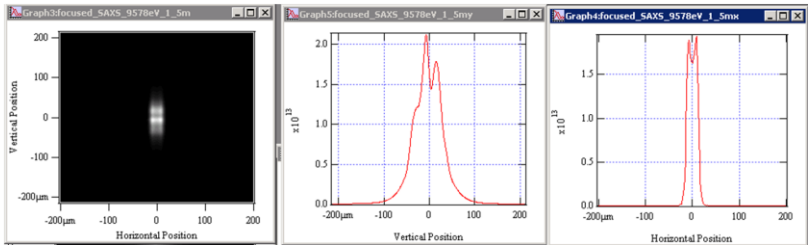


CFN group (K. Yager, J. Lhermitte et al.)

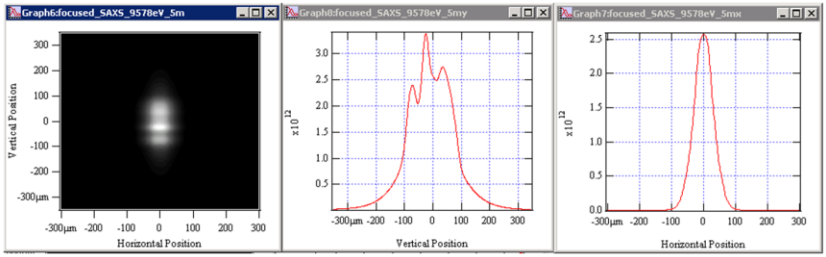
@ sample position



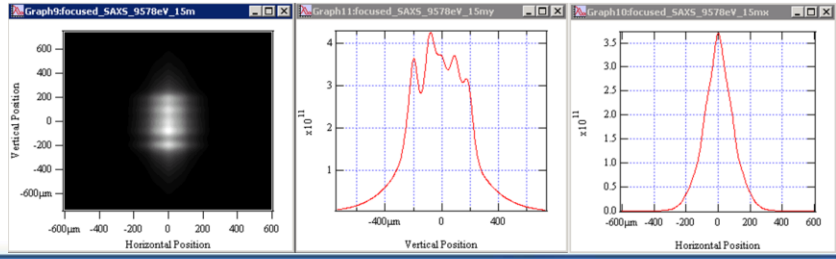
@ 1.5m downstream of sample position



@ 5.0m downstream of sample position



@ 15.0m downstream of sample position



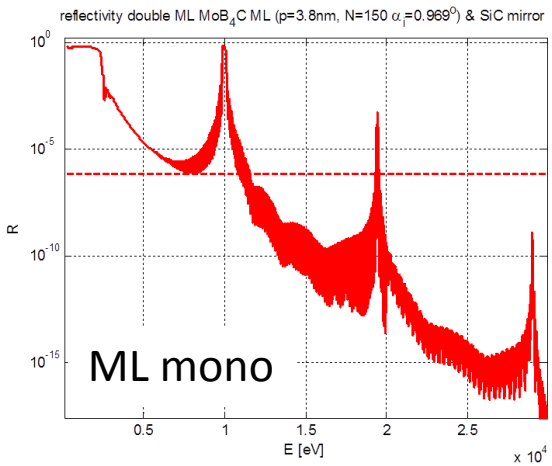
Outlook

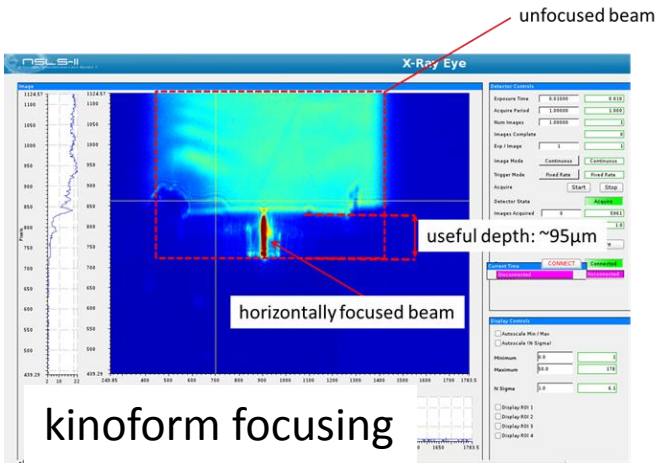
summary of wish list:

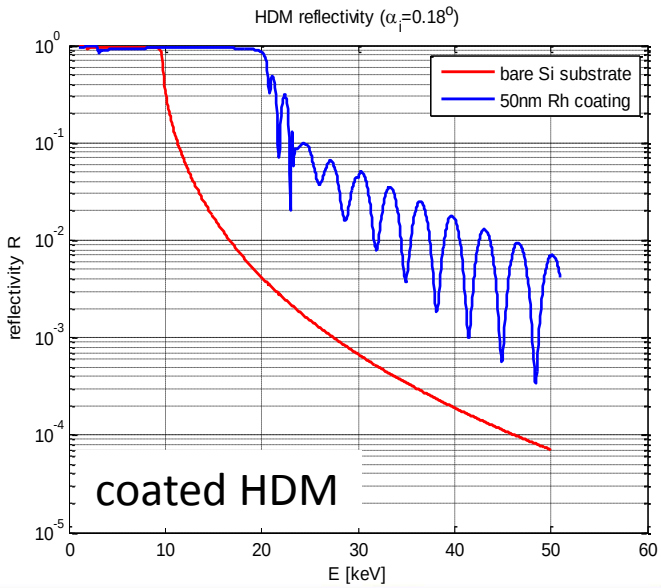
- tools for solving inverse problem for a phase object
- optical elements with vibrations
- unified, energy independent description of 'virtual' samples

Future need for CHX (some / all might exist already…):

- description of coated mirrors
- kinoform lenses
- multilayer optics
- wide-angle coherent scattering ('Bragg CDI')







Acknowledgements

The team that built and commissions two beamlines (one 'virtual', one 'real'):

- *Oleg Chubar*
- *Andrei Fluerasu*
- *Mary Carlucci Dayton*
- *Stephen Antonelli*
- *Joseph Sullivan*
- *Rick Greene*
- *Yugang Zhang*
- *Daron Chabot*
- *Diego Omitto*
- *Bruno Martins*
- *Yong Hu*
- *Kazimierz Gofron*
- *…*

D. Laundy

D. Bruhwiler