Source and Beamline Simulations

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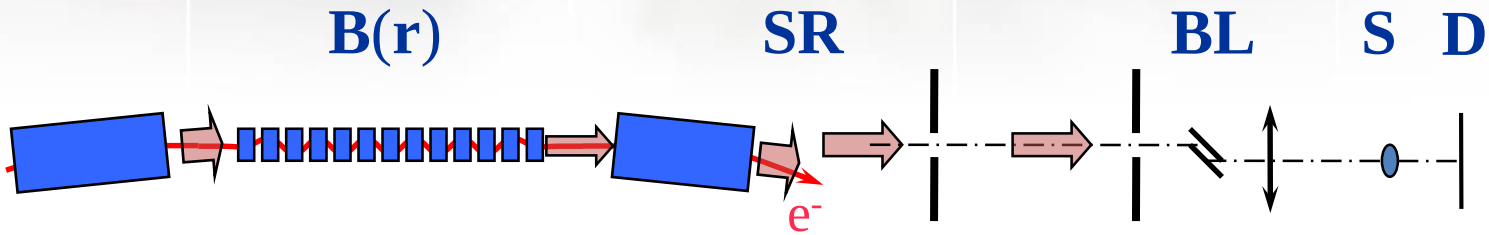
Outline

- Supported Simulation Software for Light Sources
- Radia 3D Magnetostatic Code Description
- Magnetostatic Simulations and Optimization of IDs
- SRW Code Description
- Physical Optics Simulations for NSLS-II Beamlines
- Towards Simulation of Experiments
- Summary

Electrodynamics Simulation Codes for Synchrotron Light Sources



- Computation of **magnetic fields** produced by permanent magnets, coils and iron blocks in 3d space, optimized for the design of **accelerator magnets**, **undulators** and **wigglers**

Radia code
started at ESRF in 1996

- **Sorting** and **shimming** of insertion device magnets

IDBuilder code
started at SOLEIL in 2004

- Fast computation of **synchrotron radiation** by relativistic electrons in magnetic fields of arbitrary configuration
- **Physical optics** based simulation of **radiation propagation** through a beamline, from source to sample
- Simulation of some **experiments** with **SR**

SRW code
started at ESRF in 1997; released to Open Source in 2012

Many thanks to **Pascal Elleaume** and **Jean-Louis Laclare**

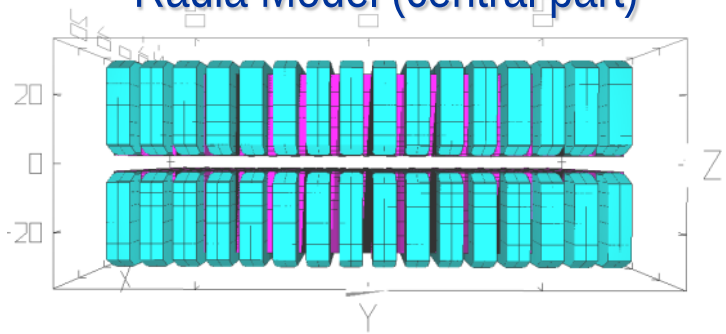
Radia – 3D Magnetostatics Code Optimized for Insertion Devices and Accelerator Magnets

- First official version of RADIA was developed at ESRF in 1996-97 (written in C++, interfaced to Wolfram Mathematica); compiled versions are distributed from: http://www.esrf.eu/Accelerators/Groups/InsertionDevices/Software/Radia
  Many thanks to Pascal Elleaume
- Radia was released to Open Source in 2018 by ESRF under BSD type license.
  Many thanks to Joel Chavanne
- The main Open Source repository, containing all C/C++ sources, C API, all interfaces and project development files, is on GitHub: https://github.com/ochubar/Radia
- Radia for Python (2.7.x and 3.x, 32- and 64-bit) cross-platform versions were released in 2018
- Radia development was partially supported by US DOE SBIR (collaboration with RadiaSoft LLC): Phase 1 successfully finished, decision about Phase 2 allocation is expected in April 2019

U.S. DEPARTMENT OF ENERGY Office of Science BROOKHAVEN NATIONAL LABORATORY radiasoft

Hybrid In-Vacuum Undulator Magnetic Performance, Acceptable Gaps and Lengths

Radia Model (central part)



IVU Parameters

Reference Geometry:

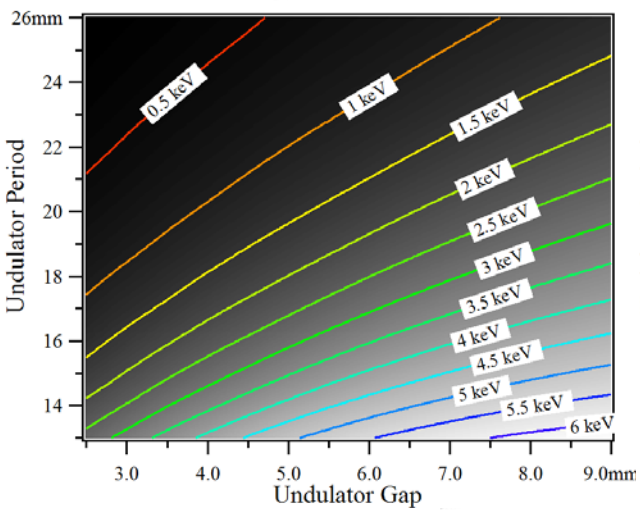
Pole Width: 40 mm
Pole Height: 25 mm
Pole Thickness: 3 mm
(for λ_u = 20 mm)

Magnet Width: 50 mm
Magnet Height: 29 mm

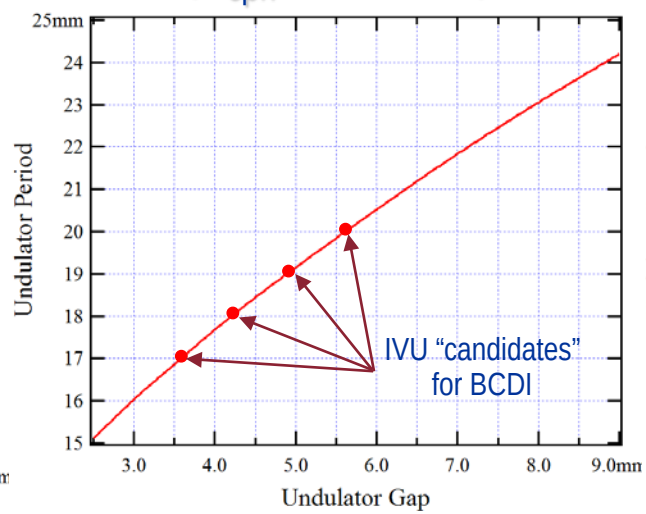
Materials:

Pole: Va Permendur
Magnet: NdFeB, Br = 1.19 T

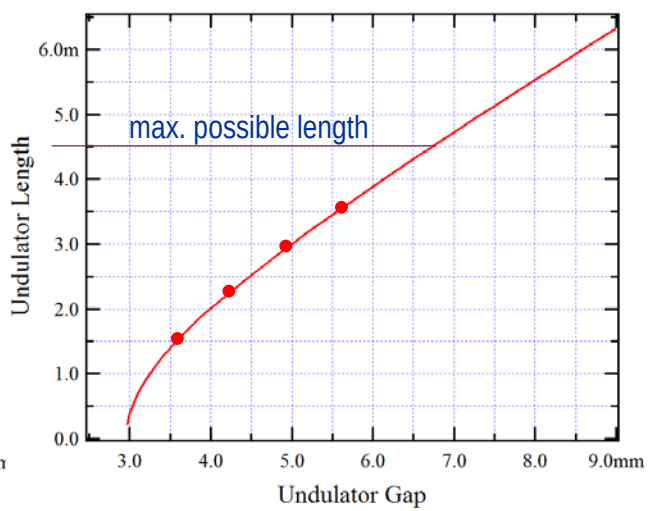
Fundamental Photon Energy vs IVU Gap and Period at E_{el} = 3 GeV



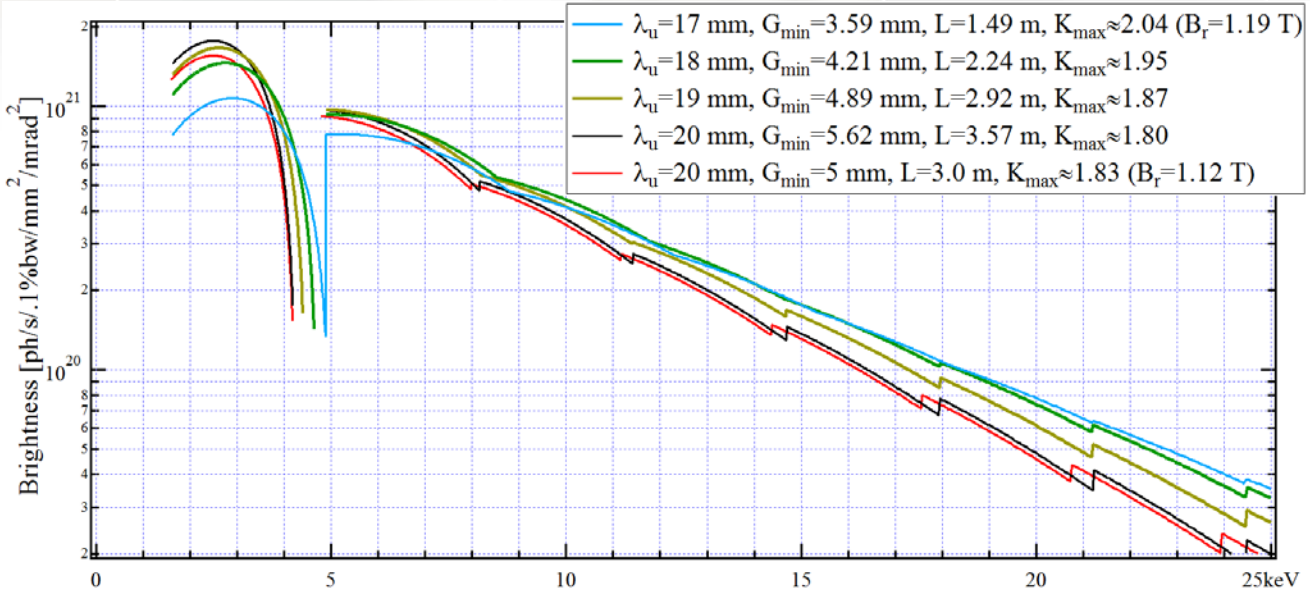
IVU Period vs Gap at E_{1ph} = 1.633 keV ($E_{3ph} \approx$ 4.9 keV)

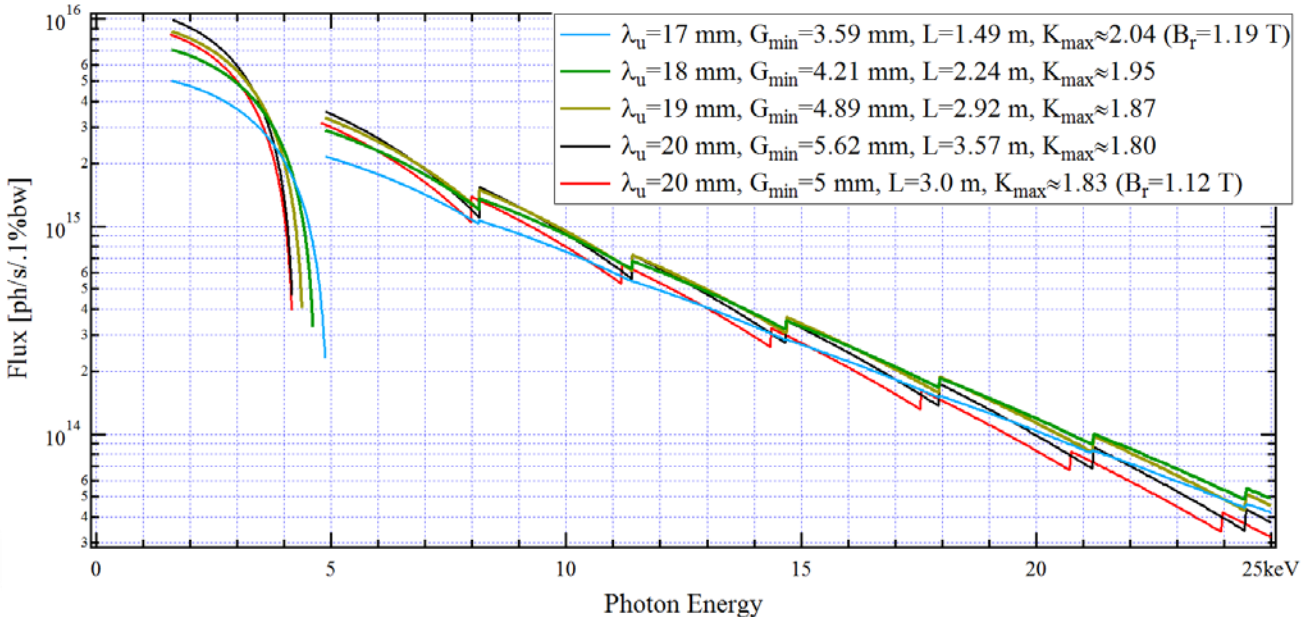


Maximal IVU Length vs Gap for Low-Beta Straight Section of NSLS-II (geom. "stay clear")



Approximate (!) Spectral Brightness and Flux at Odd Harmonics of Possible Future BCDI IVU





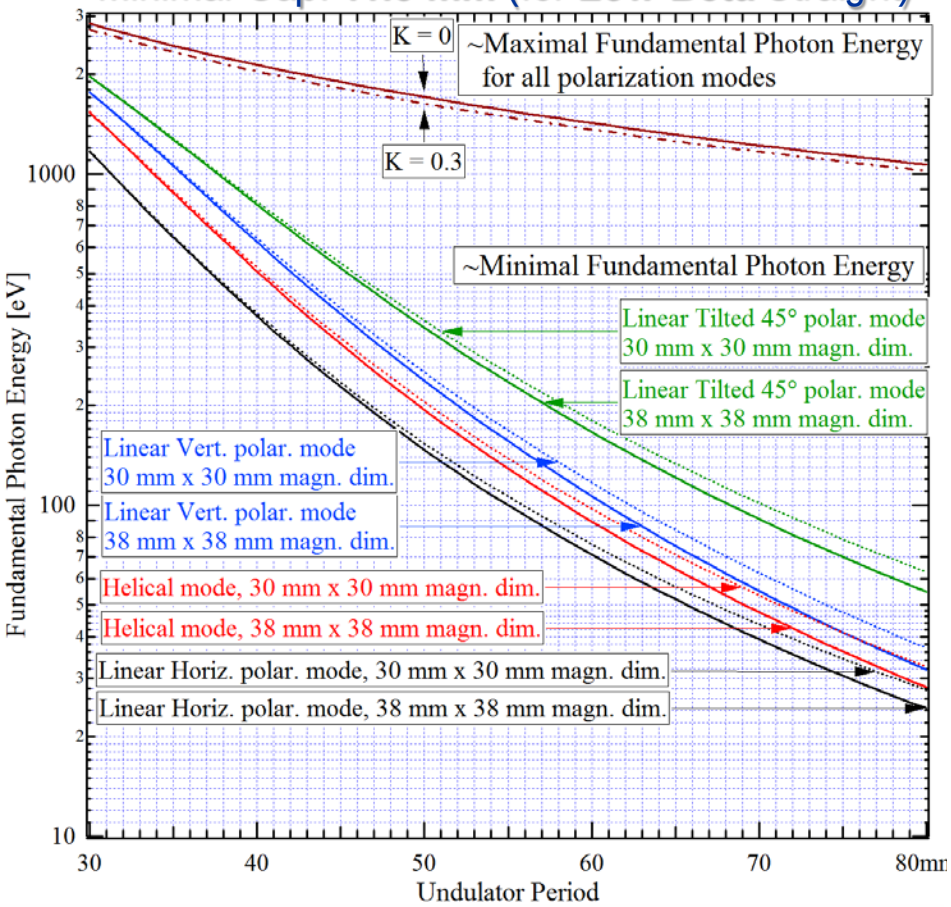
ε_x = 0.9 nm
β_{x0} = 1.84 m
ε_y = 8 pm
β_{y0} = 1.17 m

APPLE-II Elliptically-Polarizing Undulator Period Choice at NSLS-II

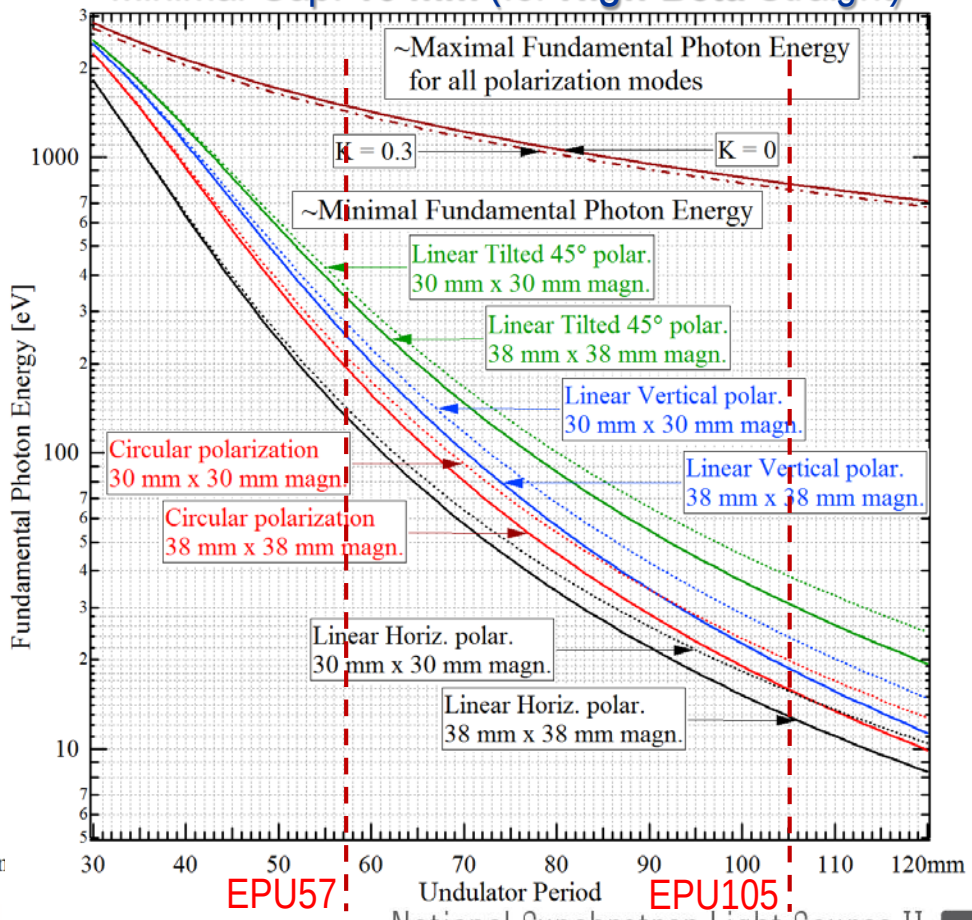
Minimal and Maximal Photon Energies of the Fundamental vs Undulator Period for E = 3 GeV

Assumption for Remnant Magnetization of NdFeB material: B_r = 1.25 T

Minimal Gap: 11.5 mm (for Low-Beta Straight)



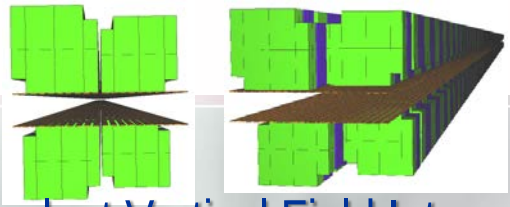
Minimal Gap: 16 mm (for High-Beta Straight)



APPLE-II structure was invented by S. Sasaki

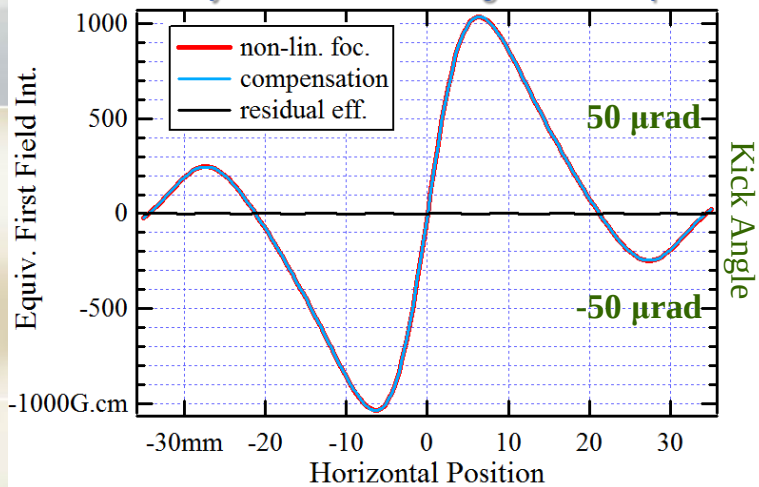
RADIA simulations

Compensation of EPU105 Nonlinear Focusing Effects by Current Strips in Linear Vertical Polarization Mode at 19 mm Gap ($E_{ph\ min} \approx 30$ eV)

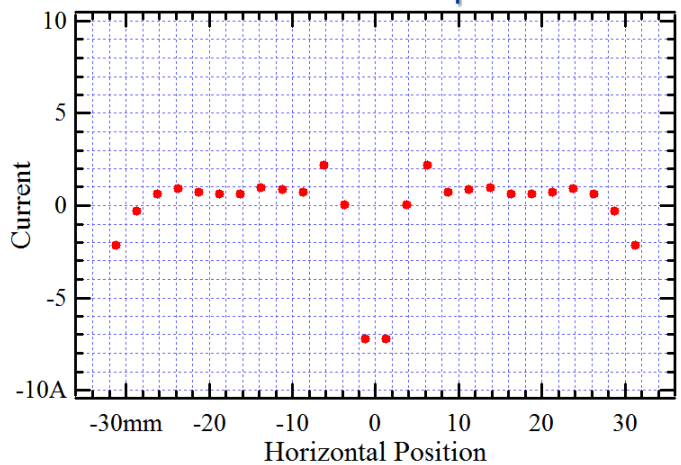


Current Strips Idea: I. Blomqvist
First Implementation: J. Bahrdt (BESSY)

Equivalent Vertical Field Integrals: Non-Linear Dynamical Focusing and Compensation



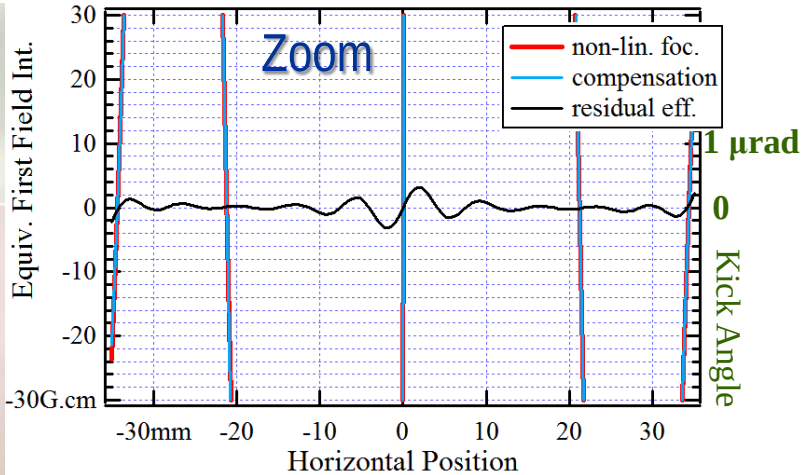
Compensating Currents in Lower Strips



Since the Dynamical Effects are Anti-Symmetric vs x:

$$\mathbf{J}_{\substack{upper\\strips}}(x) = \mathbf{J}_{\substack{lower\\strips}}(-x)$$

Number of Strips used:
2 x 26
Strip Dimensions:
2 mm x 0.3 mm x 3.2 m
Horizontal Gap bw Strips:
0.5 mm
Vertical Gap bw Strips:
15.2 mm
Max. Abs. Current:
~ 7.2 A
Estimated Joule Heating:
~ 25 W? (if R_1= 92 mΩ?)



Efficient Solving for Currents Using the Tikhonov Regularization

Field Integral (at y=0) from Currents in Strip Conductors:

$$\mathbf{I} = \mathbf{Q}\mathbf{J}$$

Matrix calculated using Radia

Currents in Strip Conductors from Field Integral (Regularized Solution):

$$\mathbf{J} = (\mathbf{Q}^T\mathbf{Q} + \mathbf{\Gamma}^T\mathbf{\Gamma})^{-1}\mathbf{Q}^T\mathbf{I}$$

Tikhonov Matrix

In these calculations, it was used:

$$\mathbf{\Gamma}^T\mathbf{\Gamma} = \alpha\mathbf{E}$$

Regularization Parameter allowing to control norm of solution (i.e. max. currents)

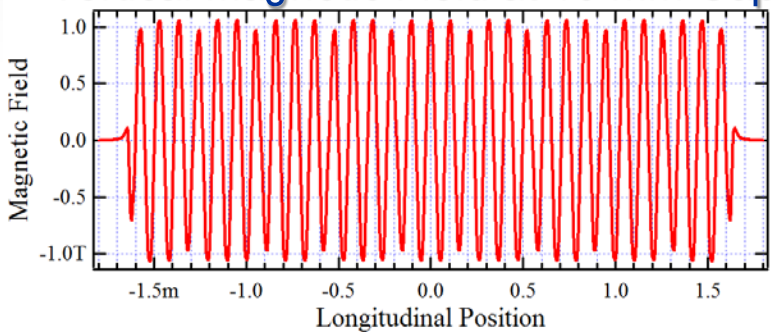
Unit Matrix

EPU105 Quasi-Periodic Option

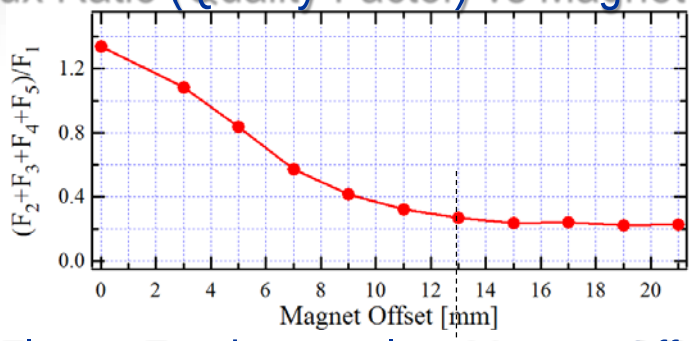
Magnet Structure

This / similar method was first used at ELETTRA (B. Diviacco) and at ESRF (J. Chavanne)

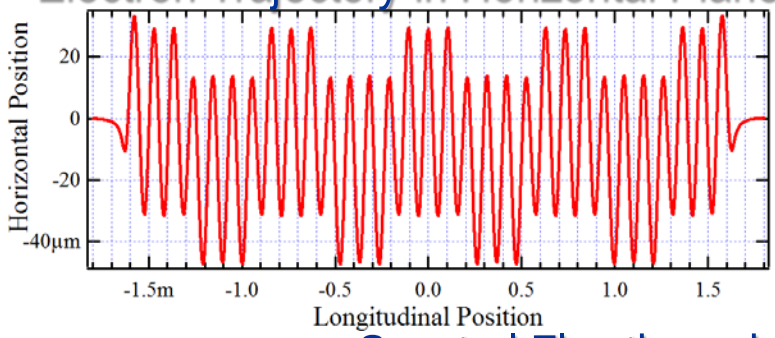
Vertical Magnetic Field at 16 mm Gap



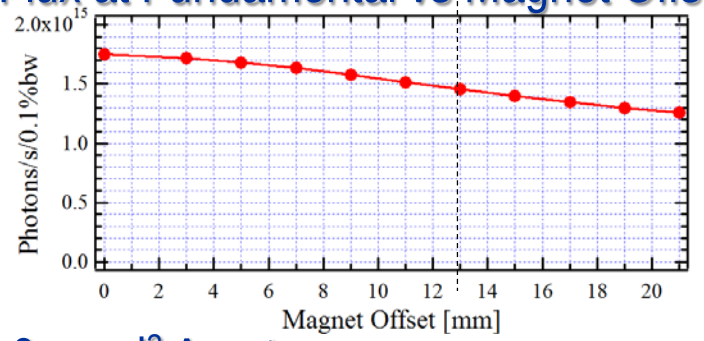
Flux Ratio (Quality Factor) vs Magnet Offset



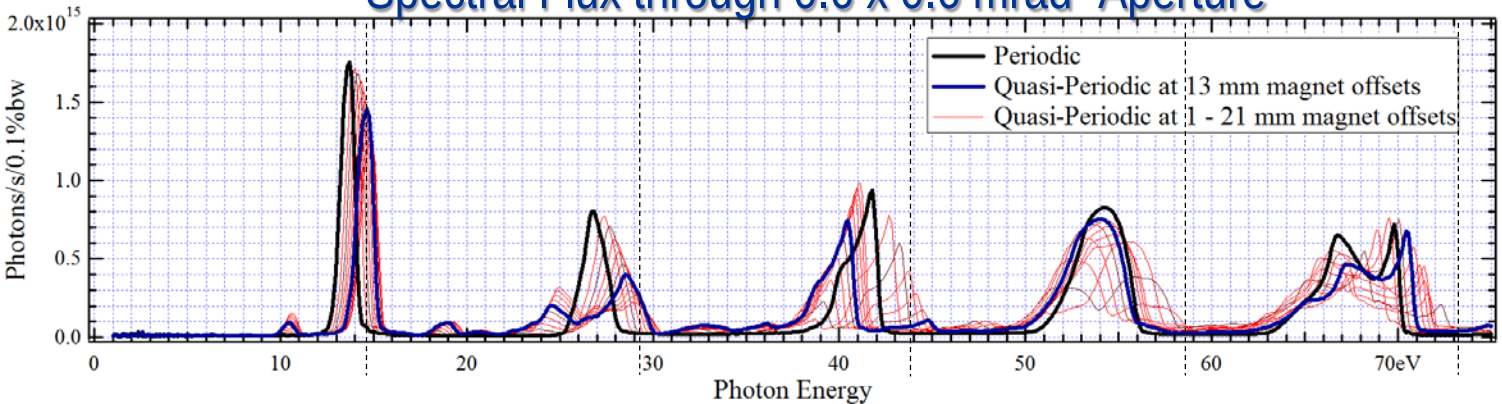
Electron Trajectory in Horizontal Plane



Flux at Fundamental vs Magnet Offset



Spectral Flux through 0.6 x 0.6 mrad^2 Aperture



EPU105 was magnetically assembled and shimmed in-house at NSLS-II using IDBuilder code.

C. Kitegi
M. Musardo

“Synchrotron Radiation Workshop” (SRW) – Physical Optics Code for SR Emission and Propagation Calculation

- First official version of SRW was developed at ESRF in 1997-98 (written in C++, interfaced to IGOR Pro); compiled versions are distributed from: http://www.esrf.eu/Accelerators/Groups/InsertionDevices/Software/SRW
  Many thanks to Pascal Elleaume
- SRW was released to Open Source in 2012 under BSD type license.

  The main Open Source repository, containing all C/C++ sources, C API, all interfaces and project development files, is on GitHub: https://github.com/ochubar/SRW
- SRW for Python (2.7.x and 3.x, 32- and 64-bit) cross-platform versions were released in 2012
- SRW development is partially supported by US DOE SBIR (collaboration with RadiaSoft LLC) and DOE “Field Work Proposal”
- SRW under Sirepo web interface is available since 2015: https://beta.sirepo.com/light#/home

Web-Based Cloud-Computing Interface to SRW and Other Codes

https://beta.sirepo.com/light#

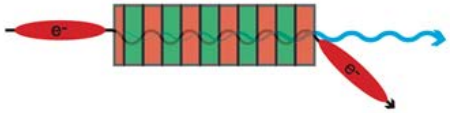
Synchrotron Radiation Workshop

To facilitate access to SR and X-Ray optics calculations for different groups of scientists and engineers, a web-based interface to SRW was developed recently.

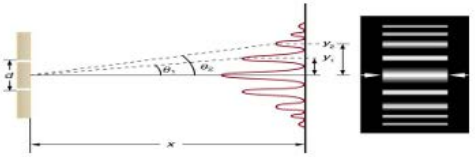
It supports both simple SR / UR / wave optics calculations, and complicated partially-coherent emission / propagation simulations for beamlines and experiments at Light Source facilities. The simulations can be driven by GUI and / or Python scripts.

Work is supported by US DOE SBIR grant and carried out by RadiaSoft LLC in collaboration with BNL / NSLS-II

Synchrotron Radiation



Wavefront Propagation

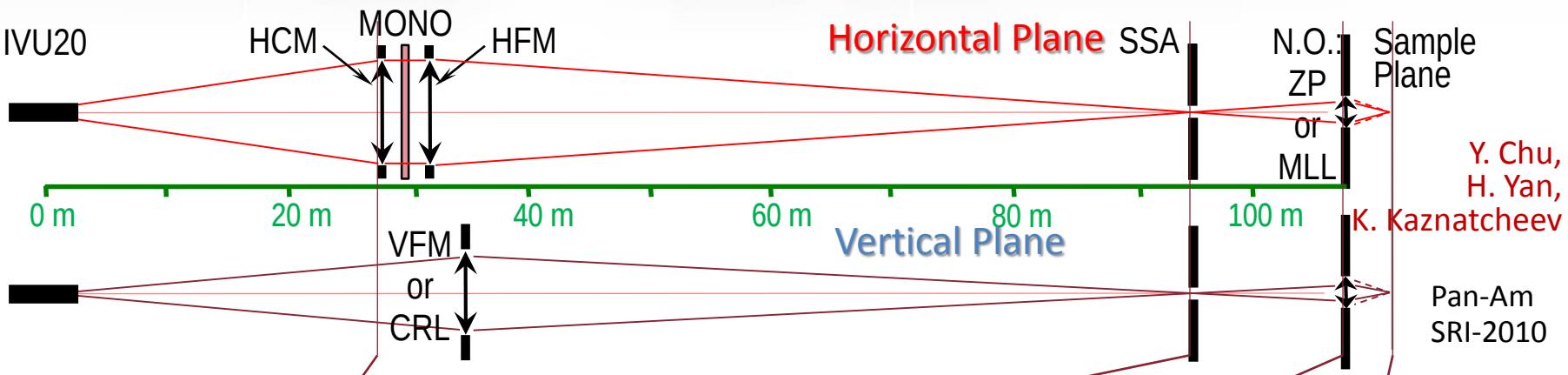


Light Source Facilities

M.S.Rakitin, P.Moeller, R.Nagler, B.Nash, D.L.Bruhwiler, D.Smalyuk, M.Zhernenkov, and O.Chubar, J. Synchrotron Rad., Vol. 25, pp. 1877-1892 (2018).

Expert users only

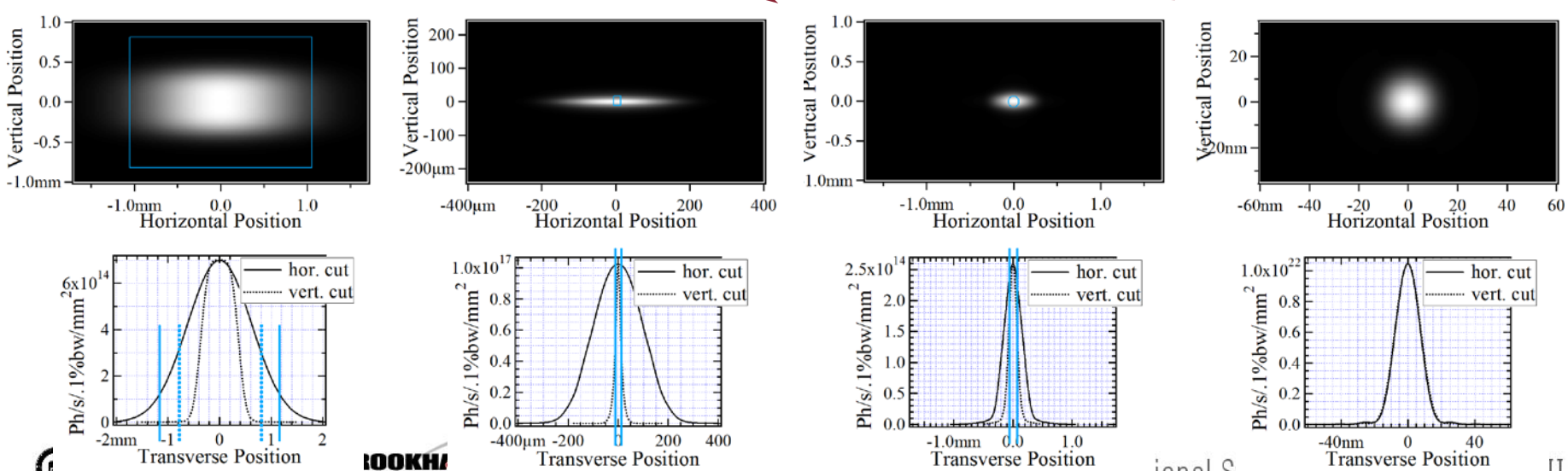
NSLS-II Hard X-Ray Nanoprobe (HXN) Beamline Optical Layout and Partially-Coherent Radiation Propagation Simulations



Flux after HCM: **~7.4x10^{14}** ph/s/.1%bw

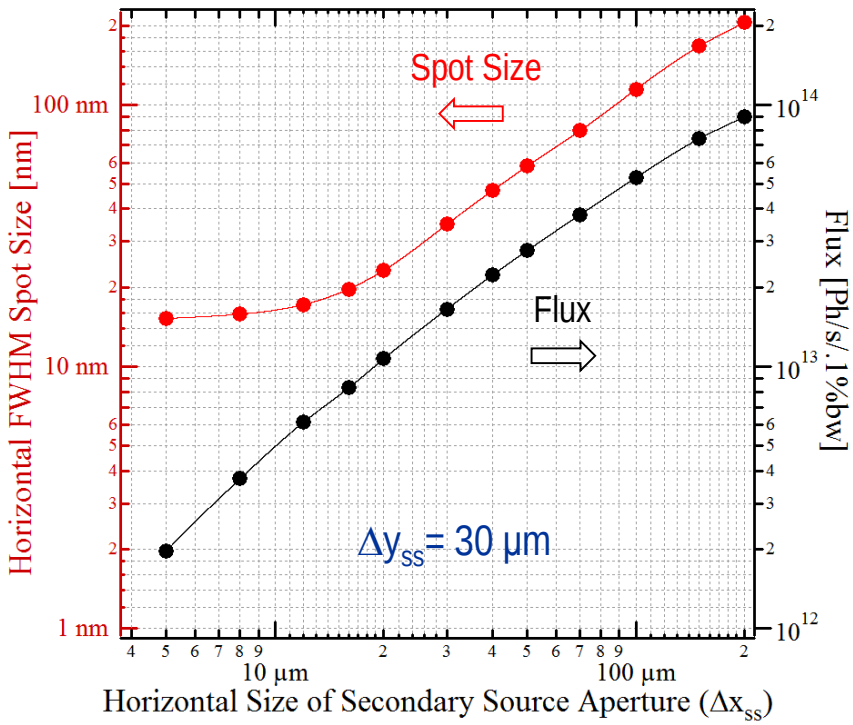
Intensity Distributions

Flux within N.O. Aperture (d=150 µm): **~3.6 x10^{12}** ph/s/.1%bw

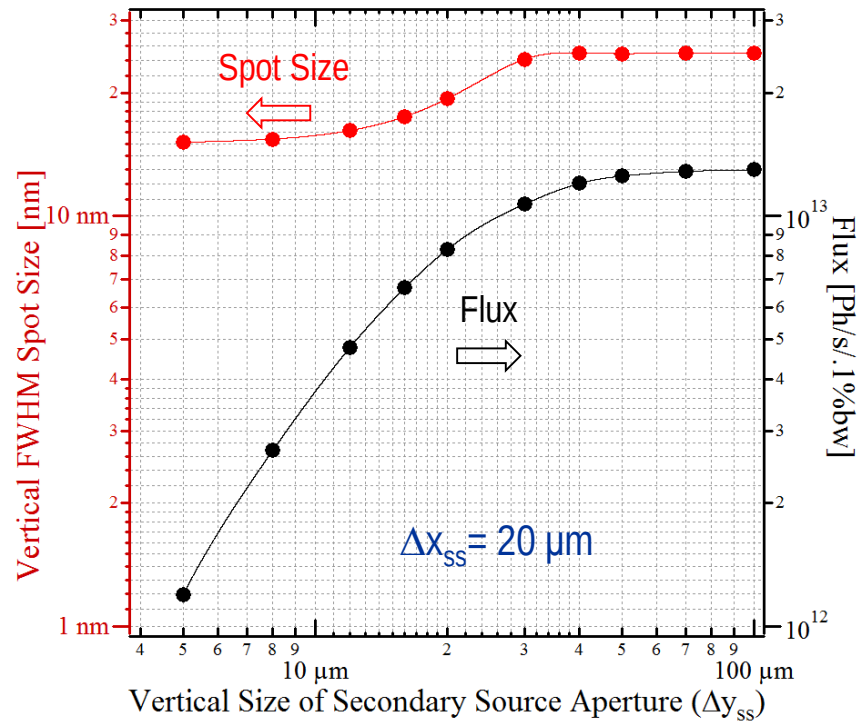


Final Focal Spot Size and Flux vs Secondary Source Aperture Size at HXN

Horizontal Spot Size and Flux
vs Horizontal Secondary Source Aperture Size



Vertical Spot Size and Flux
vs Vertical Secondary Source Aperture Size



Secondary Source Aperture located at 94 m from Undulator
Spot Size and Flux calculated for Nanofocusing Optics simulated by Ideal Lens
with F = 18.14 mm, D = 150 µm located at 15 m from Secondary Source (109 m from Undulator)

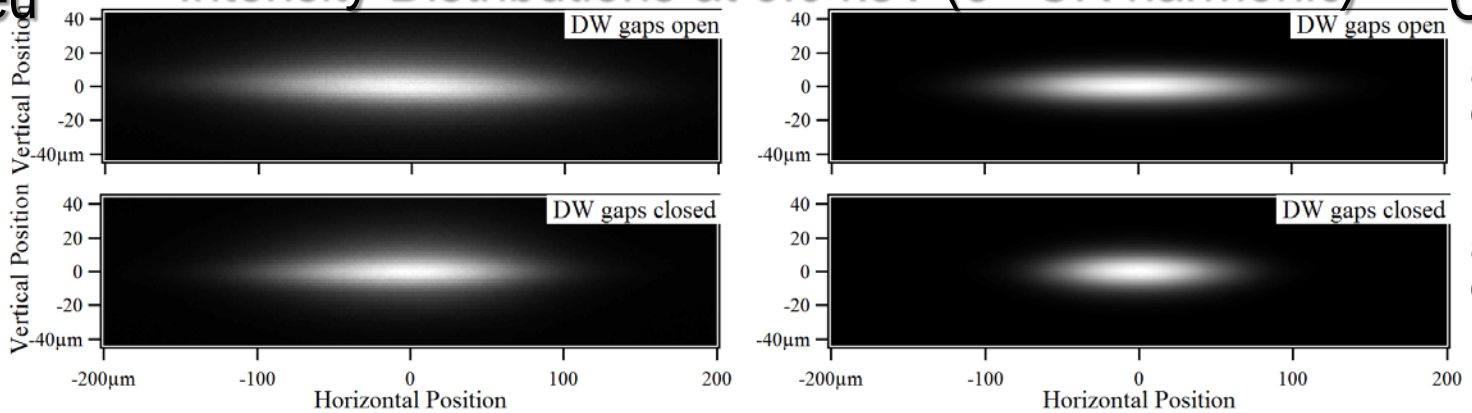
Electron Beam Imaging Near Secondary Source Aperture (at ~63 m from undulator) of HXN Beamline

Intensity Distributions at 8.0 keV (5th UR harmonic)

Measured | **Calculated**

DW Gaps Open

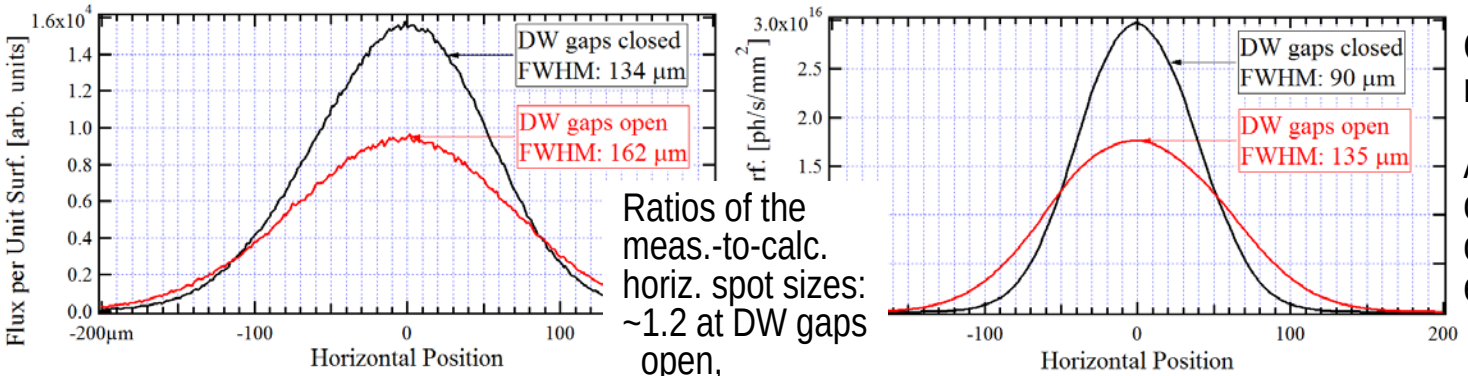
DW Gaps Closed



$\varepsilon_x \approx$ 2.1 nm
$\sigma_{ex} \approx$ 61 µm

$\varepsilon_x \approx$ 0.9 nm
$\sigma_{ex} \approx$ 40 µm

Cuts by Horizontal Mid-Plane



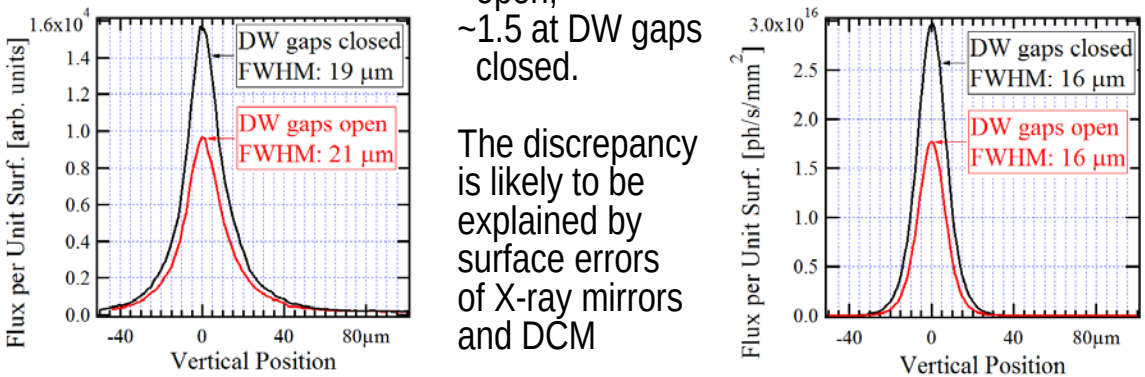
Optical magn. ~0.93

Assumption of error-free optical elements

Ratios of the meas.-to-calc. horiz. spot sizes: ~1.2 at DW gaps open, ~1.5 at DW gaps closed.

The discrepancy is likely to be explained by surface errors of X-ray mirrors and DCM

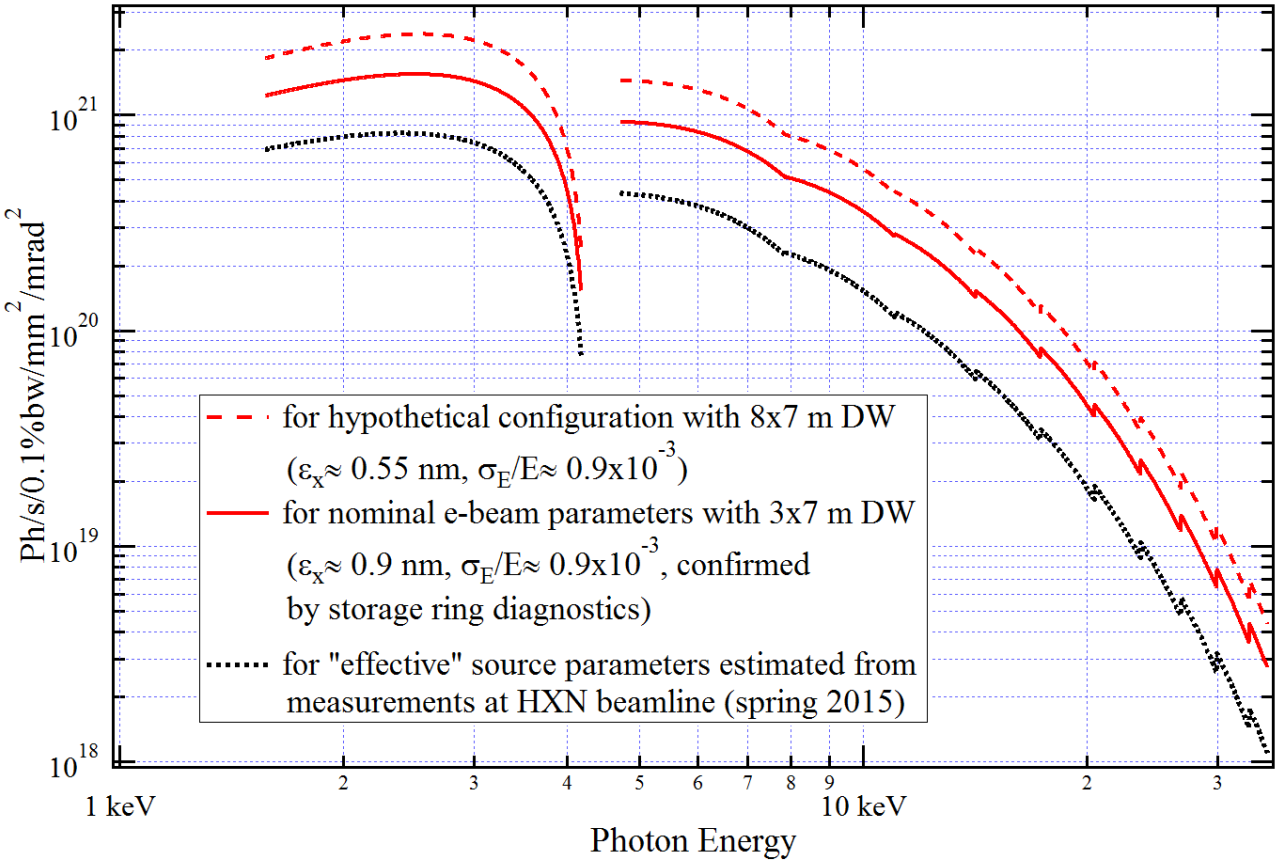
Cuts by Vertical Mid-Plane



$\varepsilon_y \approx$ 30 pm
$\sigma_{ey} \approx$ 5.9 µm

NSLS-II Brightness: Nominal and Estimated from Measurements at HXN

Approximate Spectral Brightness of IVU20 in Low-Beta Straight Section of NSLS-II



All curves are scaled for 0.5 A e-beam current.

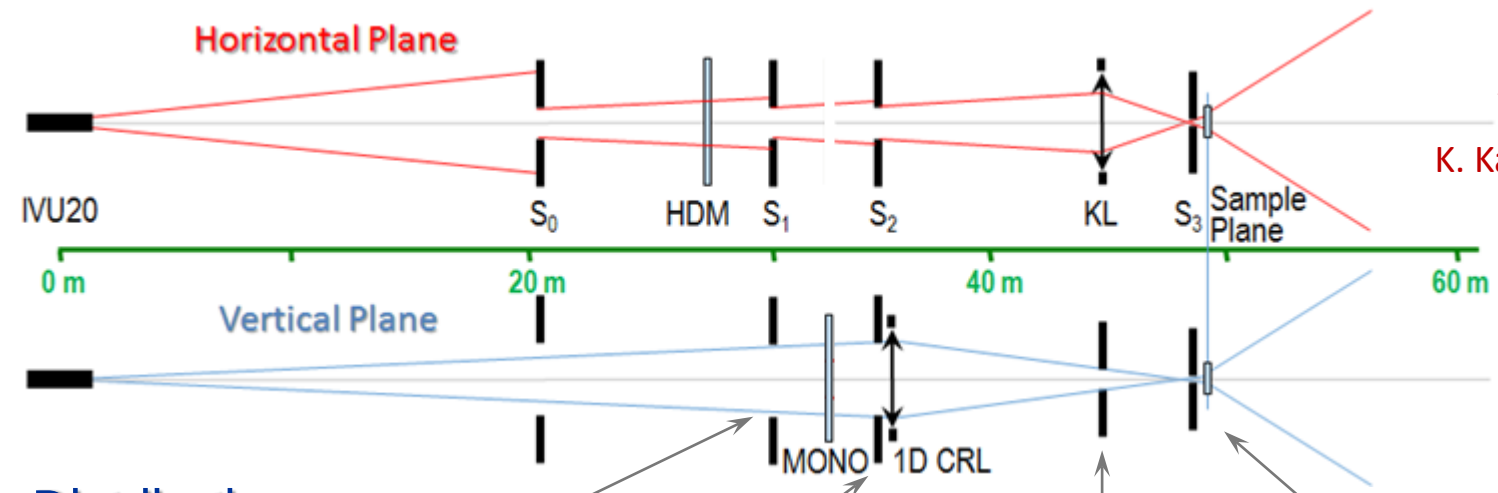
Note: absolute values of spectral brightness may not be very accurate, however, relative "locations" of the curves are credible.

The reduction of apparent brightness "observed" at the beamline is mainly attributed to imperfections of X-ray optics (horizontally-focusing bendable mirrors, monochromator, vertically-focusing CRL).

It may be possible to "restore" this apparent brightness in the future (by further fine tuning / processing / replacing of individual beamline components, identified from simulations and dedicated measurements).

NSLS-II Coherent Hard X-Ray (CHX) Beamline Optical Layout and Part.-Coherent Simulations

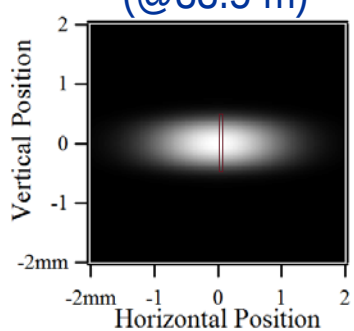
A. Fluerasu
L. Wiegart
K. Kaznatcheev



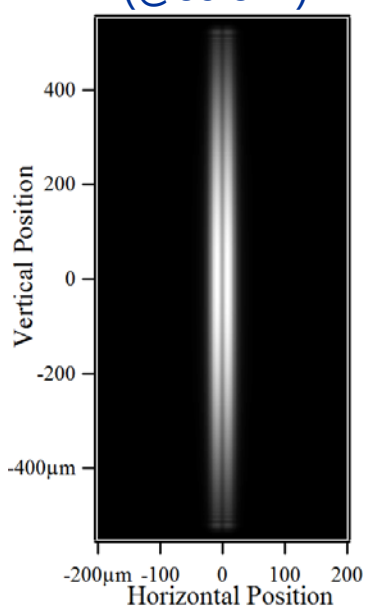
Intensity Distributions

for E = 10 keV
ΔS_{1x} = 44 µm
ΔS_{1y} = 1 mm

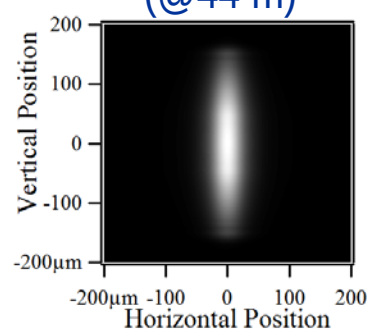
Before SS1 (@33.5 m)



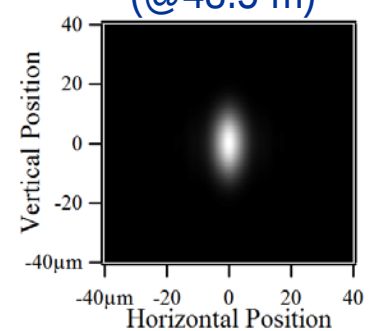
Before CRL (@35.8 m)



Before KL (@44 m)



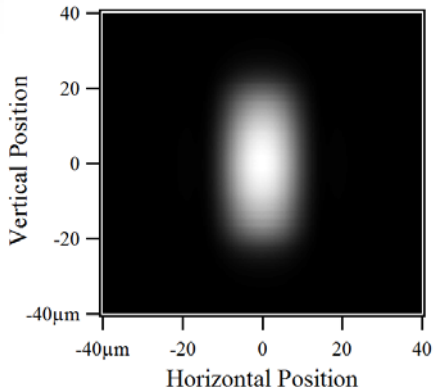
At Sample (@48.5 m)



Flux: 10^{13} ph/s/.1%bw

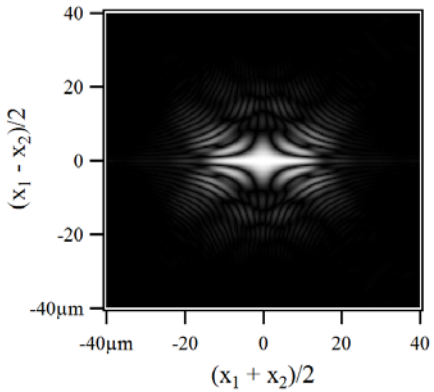
Tracking Intensity and Degree of Transverse Coherence at CHX Sample

Intensity Distribution

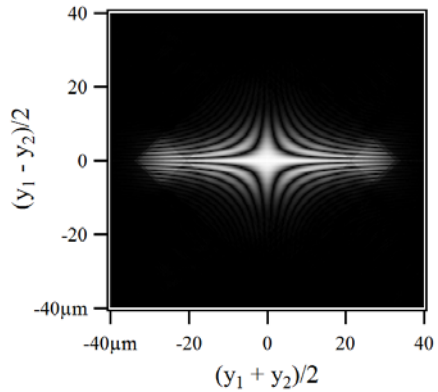


Degree of Transverse Coherence

In Horizontal Mid-Plane

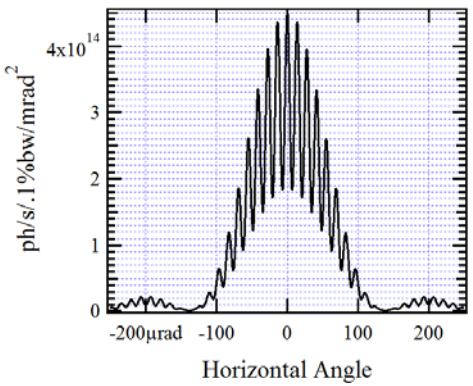


In Vertical Mid-Plane



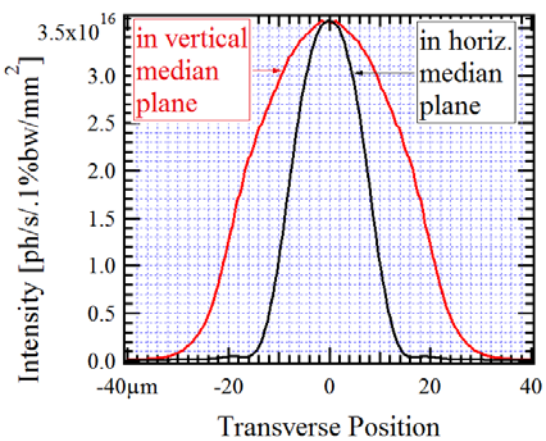
Angular Intensity (far field) after Two Slits separated by 10 µm

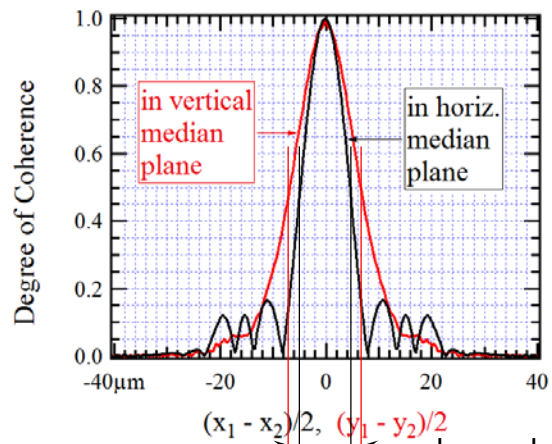
In Horizontal Plane (after vertical slits)



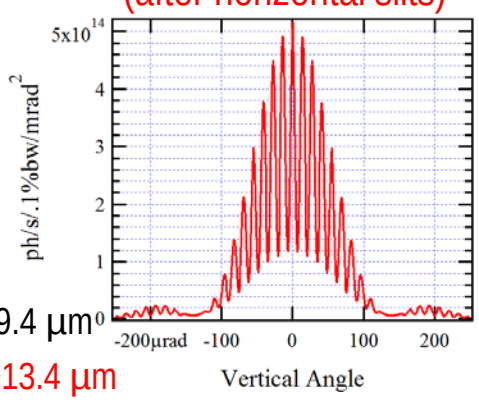
$$\mu(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega) = |M(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega)|/[M(\boldsymbol{r}_1,\boldsymbol{r}_1,\omega)M(\boldsymbol{r}_2,\boldsymbol{r}_2,\omega)]^{1/2}$$

$$M(\boldsymbol{r}_1,\boldsymbol{r}_2,\omega) \sim < \mathbf{E}_\perp(\boldsymbol{r}_1,\omega)\mathbf{E}_\perp^*(\boldsymbol{r}_2,\omega) >$$





In Vertical Plane (after horizontal slits)



hor. coherence length: ~9.4 µm

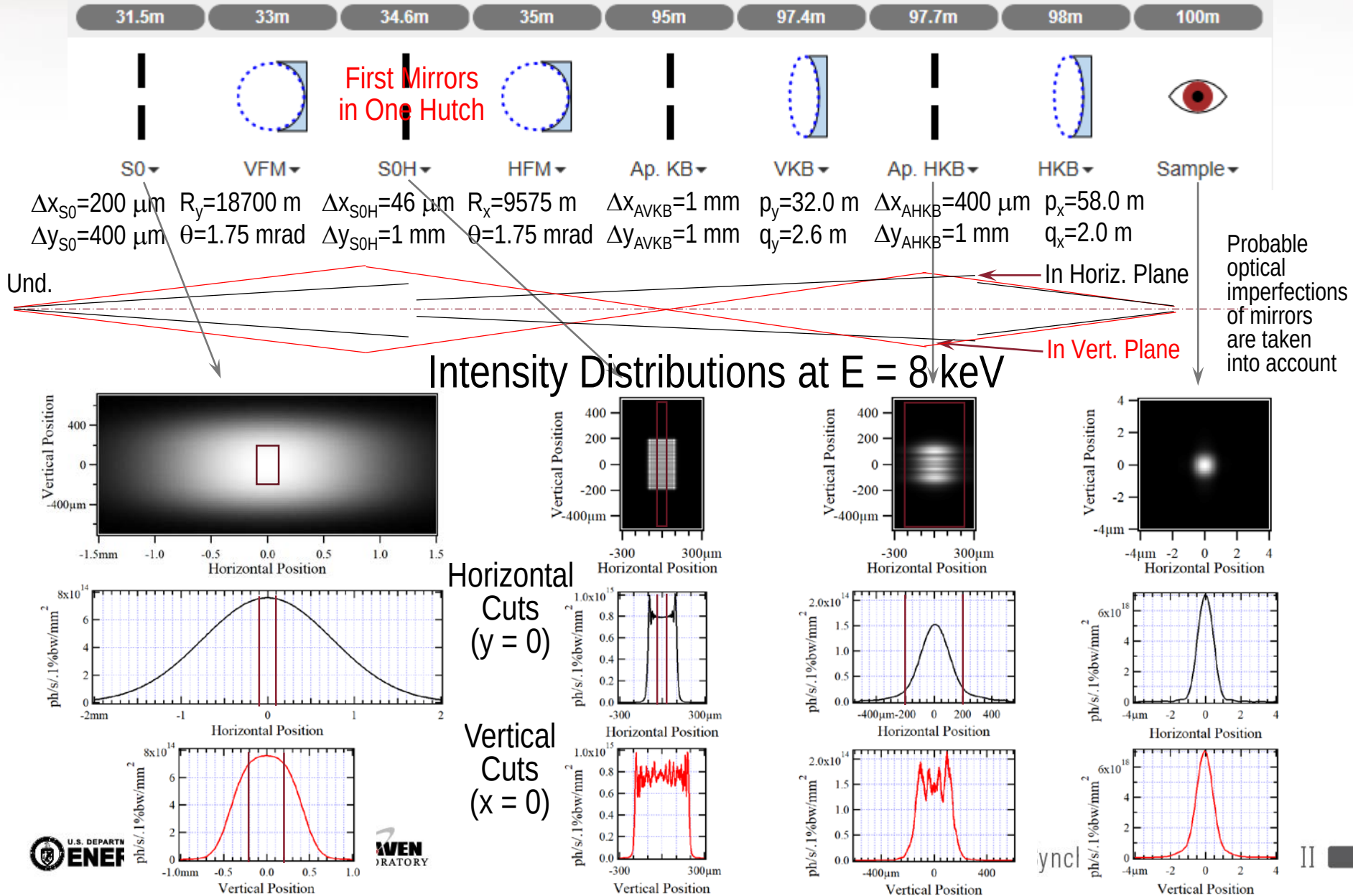
vert. coherence length: ~13.4 µm

Good agreement with 2-slit interference simulation results

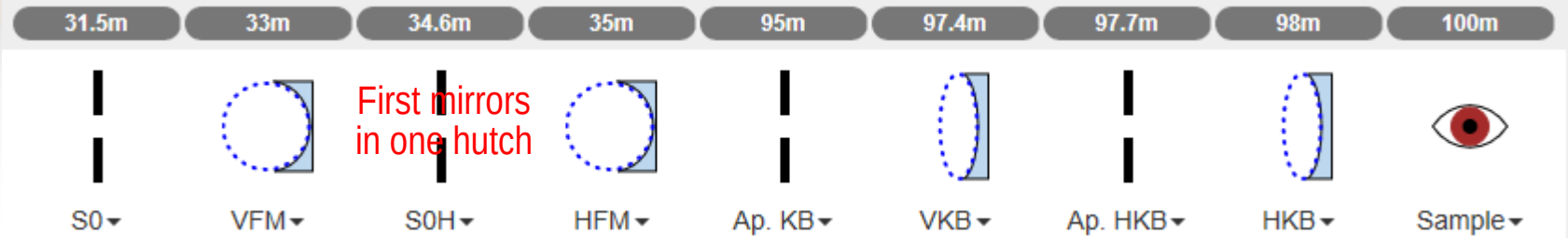
Optical Layout Considered for Bragg CDI Beamline

Long Beamline Option, settings for 1 µm Spot

G. Williams
I. Robinson



Long BL for 1 µm Spot: Intensity Distr. near Sample



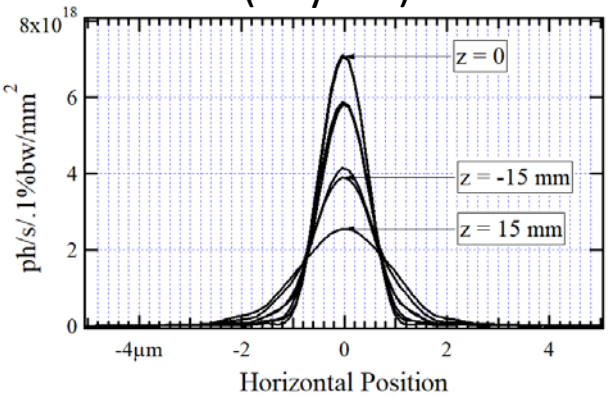
Δx_{S0}=200 µm R_y=18.7 km Δx_{S0H}=46 µm R_x=9.575 km Δx_{AVKB}=1 mm p_y=32.0 m Δx_{AHKB}=400 µm p_x=58.0 m

Δy_{S0}=400 µm θ=1.75 mrad Δy_{S0H}=1 mm θ=1.75 mrad Δy_{AVKB}=1 mm q_y=2.6 m Δy_{AHKB}=1 mm q_x=2.0 m

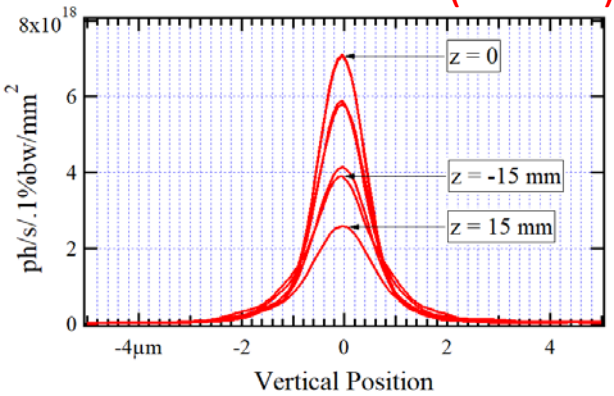
E = 8 keV

Intensity Distribution Cuts

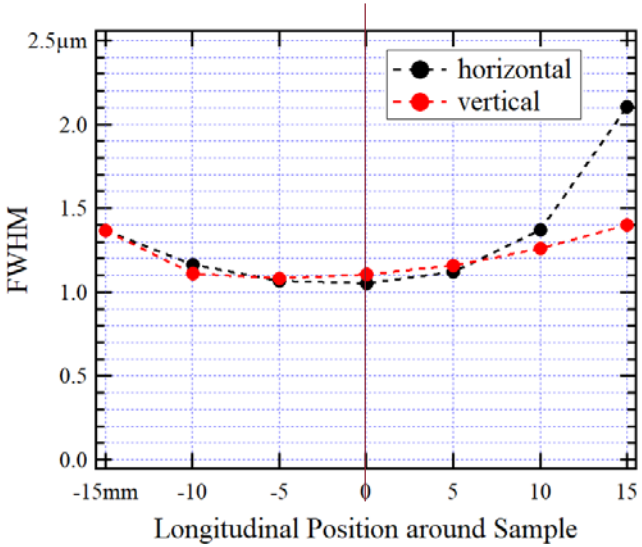
Horizontal (at y = 0)



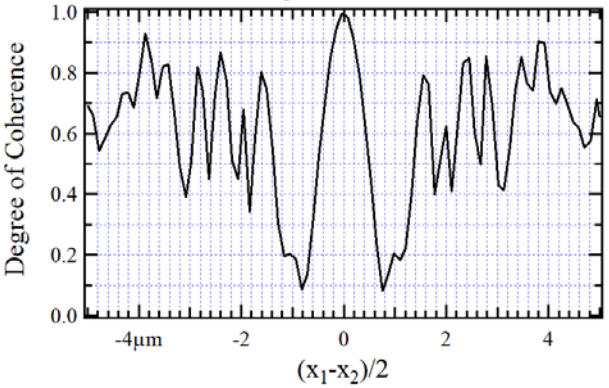
Vertical (at x = 0)

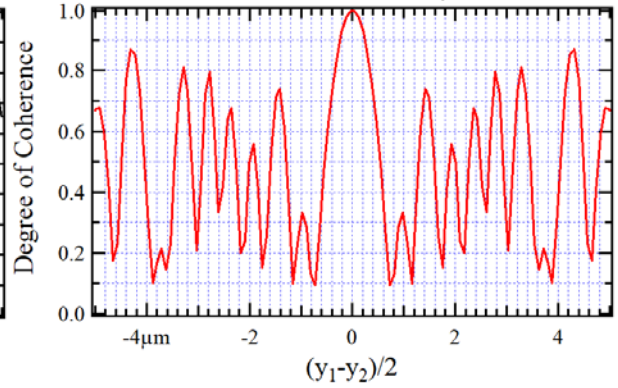


Spot Size near Sample



Degree of Coherence at Sample



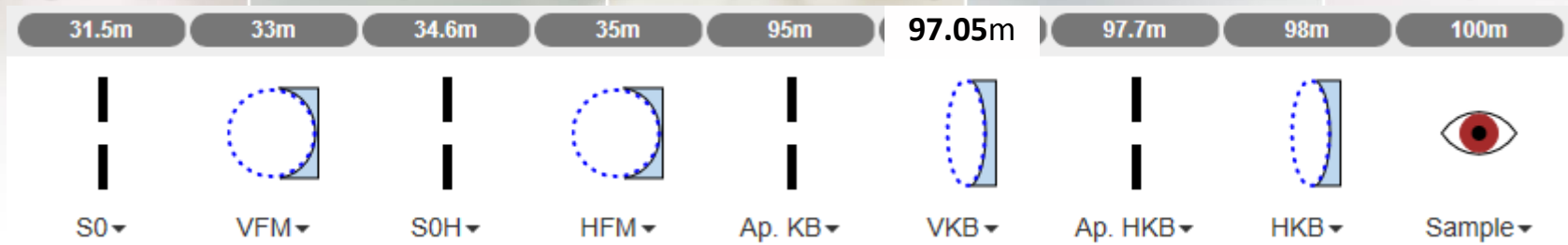


Transverse Coherence Lengths at Sample:

$l_{coh\ x} \approx$ 1.0 µm, $l_{coh\ y} \approx$ 1.1 µm

Flux: ~1.0x10^{13} ph/s/.1%bw

Long BL for 10 µm Spot: Intensity Distr. near Sample (II)



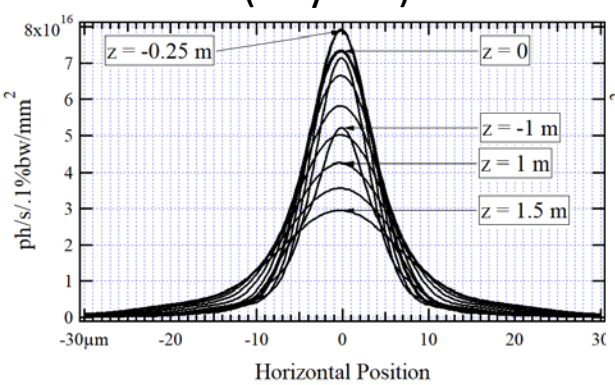
Δx_{S0}=400 µm R_y=23.6 km Δx_{S0H}=1 mm R_x=37.0 km Δx_{AVKB}=1 mm p_y=32.0 m Δx_{AHKB}=35 µm p_x=58.0 m

Δy_{S0}=800 µm θ=1.75 mrad Δy_{S0H}=1 mm θ=1.75 mrad Δy_{AVKB}=45 µm q_y=2.6 m Δy_{AHKB}=1 mm q_x=2.0 m

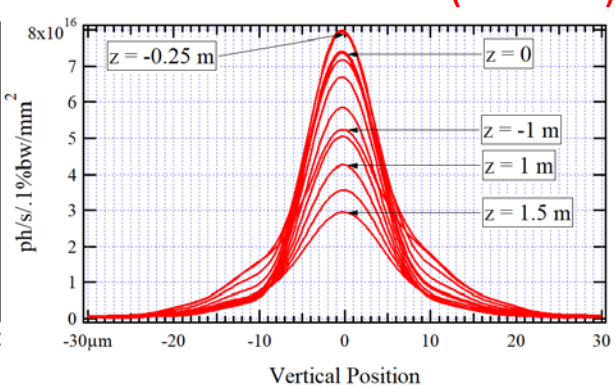
E = 8 keV

Intensity Distribution Cuts

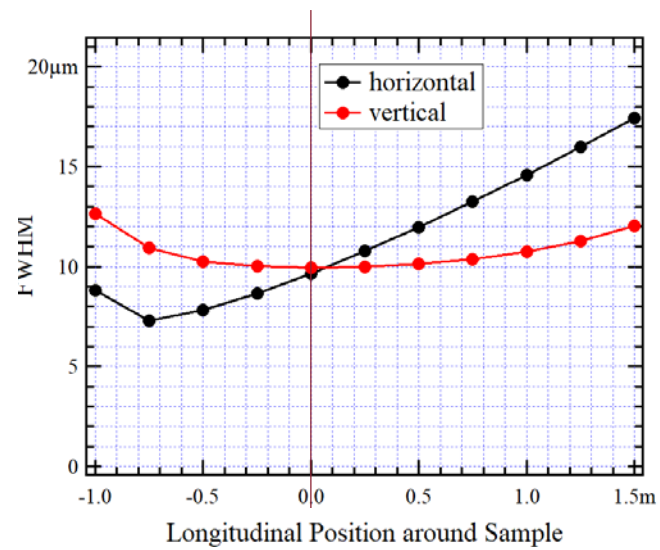
Horizontal (at y = 0)



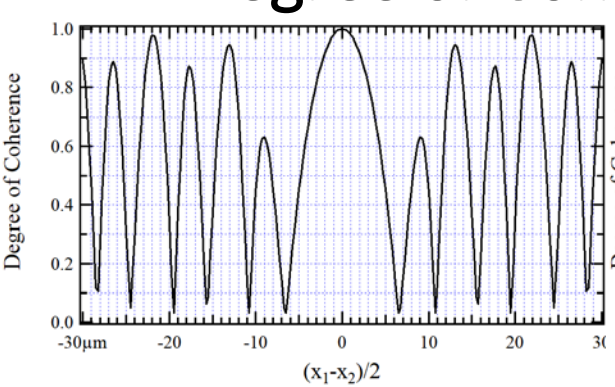
Vertical (at x = 0)

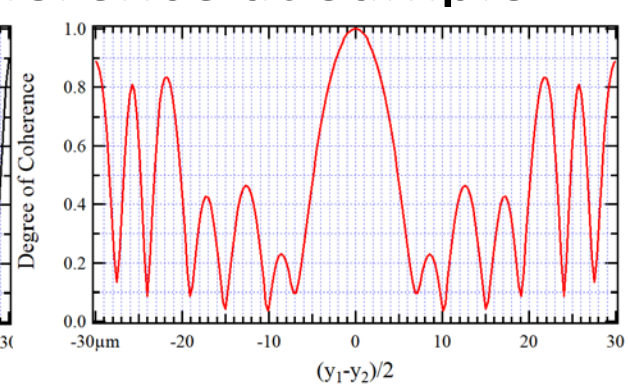


Spot Size near Sample



Degree of Coherence at Sample





Transverse Coherence Lengths at Sample:

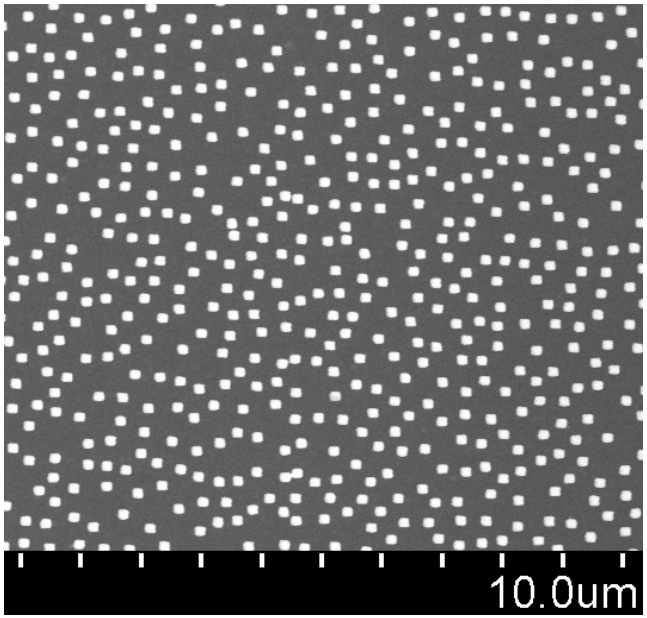
$l_{coh\ x} \approx$ 9.6 µm, $l_{coh\ y} \approx$ 9.8 µm

Flux: ~9.8x10^{12} ph/s/.1%bw

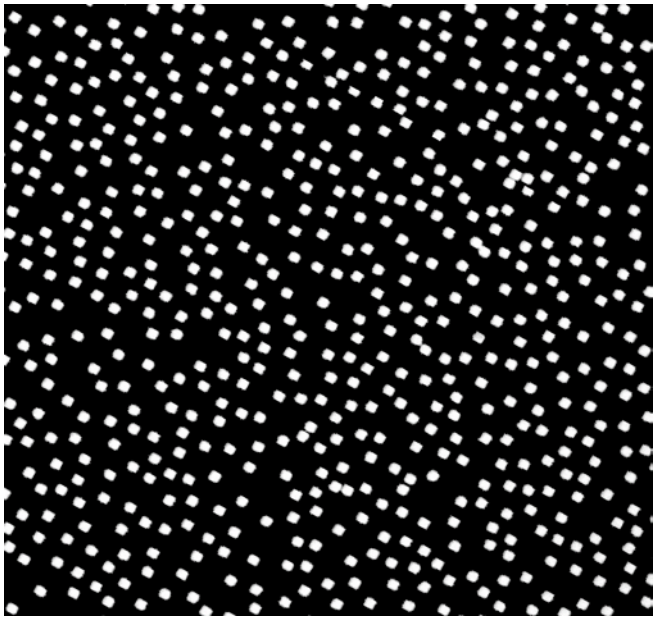
Simulation of Coherent Scattering Experiments (CHX): Processing Electron Microscope Images of Samples for Automatic Conversion to SRW Transmission Obj.

M. Rakitin

Original EM Image



Processed Image

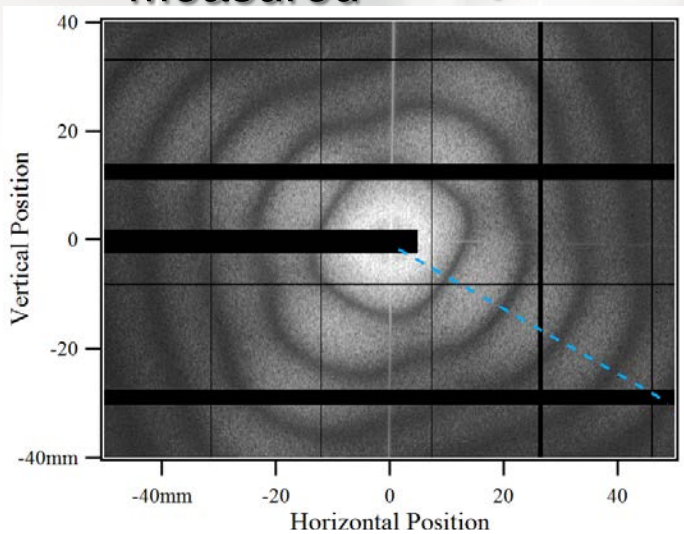


Original electron microscope image of the “random rectangular Au dots” sample fabricated at the Center of Functional Nanomaterials of BNL. The Au layer thickness is ~50 nm.

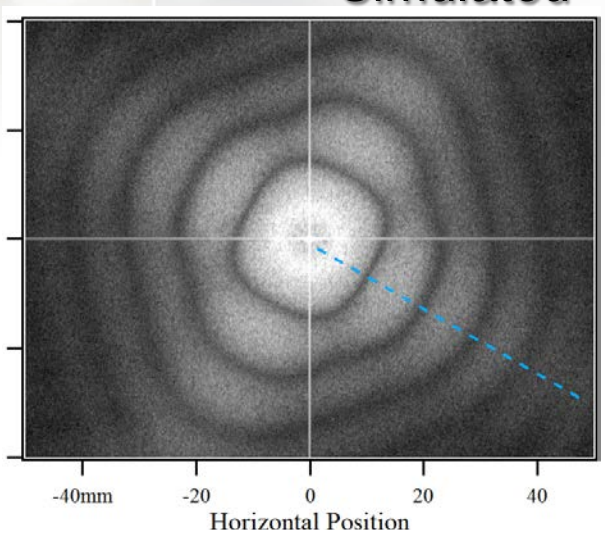
Processed and rotated image was used as input for definition of a Transmission object for SRW simulation. Rotation was added to simulate sample orientation used in the actual experiment.

Simulation of Coherent Scattering Experiments (CHX): Speckle Patterns

Measured



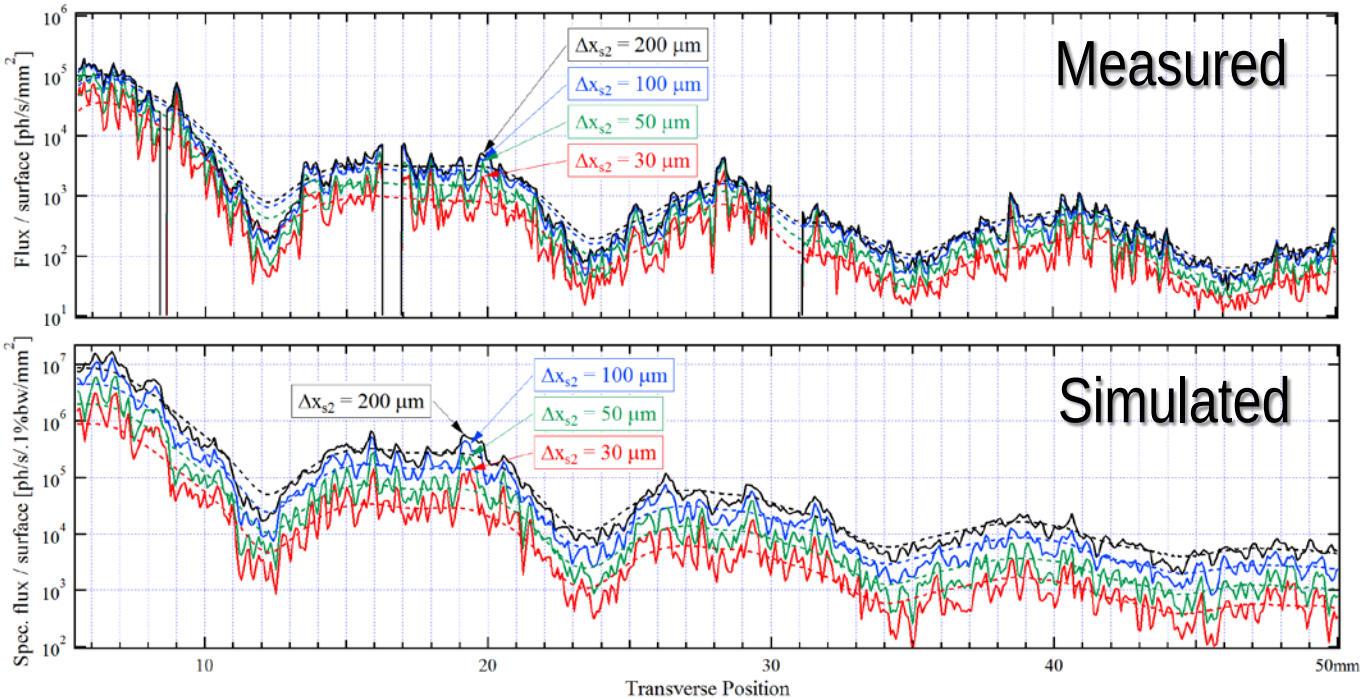
Simulated



E_{ph} = 9.65 keV

Hor. Slit Sizes:
Δx_{S2}= 50 µm
Δx_{KL}= 60 µm

Intensity along dashed lines:



Measurements were done using EIGER X 4M detector (2070x 2167 pixels of 75 µm size) located at ~16 m from sample.

A. Fluerasu
L. Wiegart
M. Rakitin

Summary

- **High-accuracy calculations** in the areas of **ID design**, **synchrotron emission**, **radiation propagation** through beamline optics, and **interaction with samples** in **coherent scattering** and some other types of **experiments**, **can be done** for the current and future light sources, using the **existing computer codes**.
- These calculations can greatly help to obtain **maximal benefits from new high brightness and high coherence ultra-low-emittance synchrotron sources** and **XFELs** in user experiments.

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