Applications of High-Accuracy Calculations for Design and Commissioning of Insertion Devices and X-Ray Optics for Beamlines at a Low-Emittance SR Source

O. Chubar, BNL, NSLS-II

70 YEARS OF DISCOVERY

A CENTURY OF SERVICE

U.S. DEPARTMENT OF ENERGY

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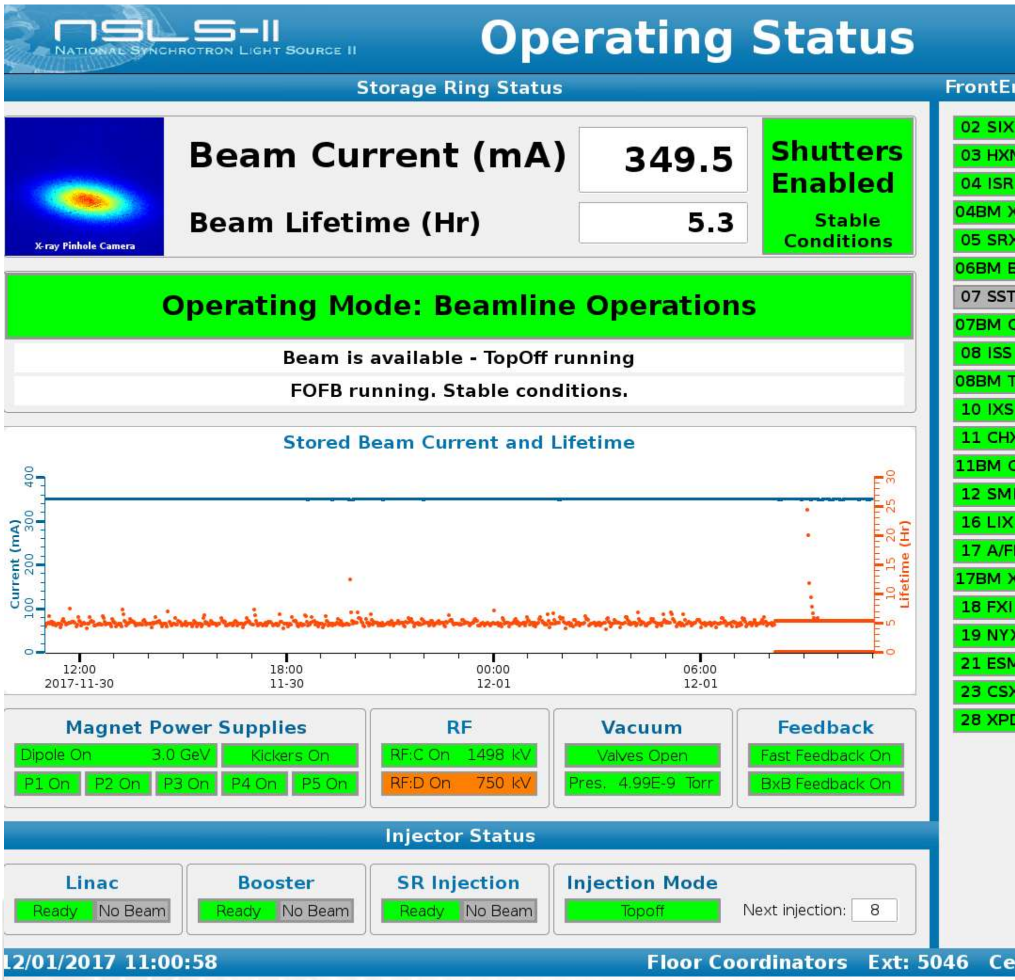
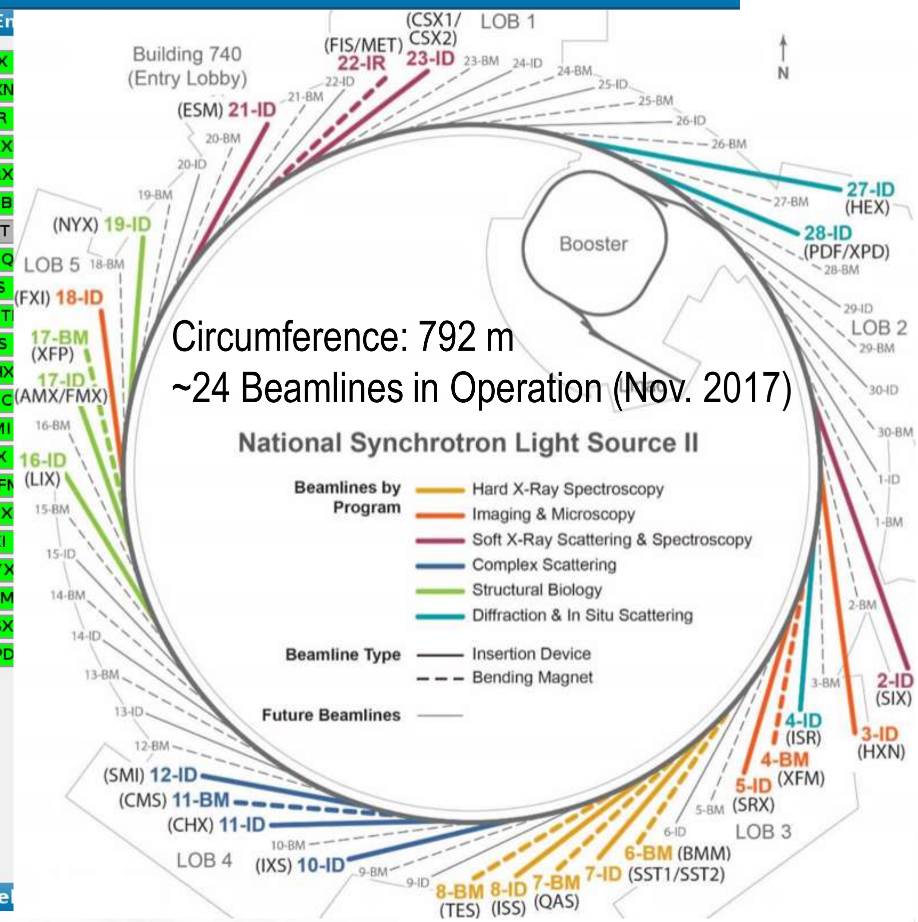
PHANGS Workshop, ELETTRA, Trieste, 4-5 December 2017

Outline

- NSLS-II is in Successful Operation since 2015
- Computer Codes for IDs and X-ray Optics
- Parametric Optimization and Spectrum-Based Alignment of IVU
- Parametric Optimization and Spectrum Characterization of (Quasi-Periodic) APPLE-II
- X-ray Optics Optimization and Performance Characterization
- Towards Complete Simulation of Experiments
- Summary

NSLS-II, a Reliable 0.9 nm Emittance 3 GeV Synchrotron Radiation Source





Circumference: 792 m

~24 Beamlines in Operation (Nov. 2017)

S. Krinsky, S. Dierker, J. Hill,
J. Murphy, F. Willeke, T. Shaftan
et al.

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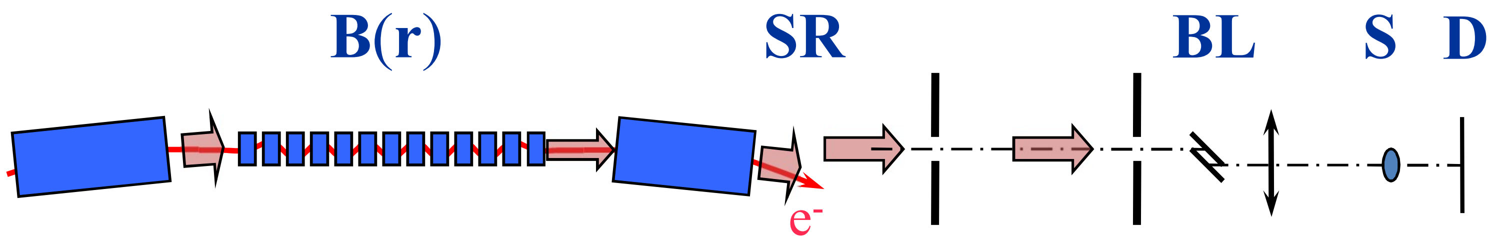
Electrodynamics Simulation Codes for Synchrotron Light Sources



- 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

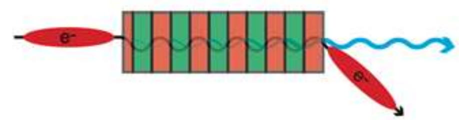
Web-Based Cloud-Computing Interface to SRW and Other Codes

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

Synchrotron Radiation Workshop

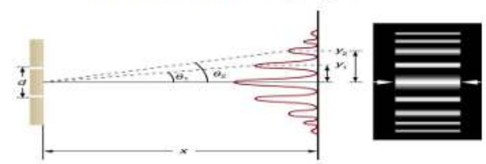
To facilitate access to SR and X-Ray optics calculations for different groups of scientists and engineers, a web-based interface to SRW was developed recently.

Synchrotron Radiation



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.

Wavefront Propagation



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

Light Source Facilities

Expert users only

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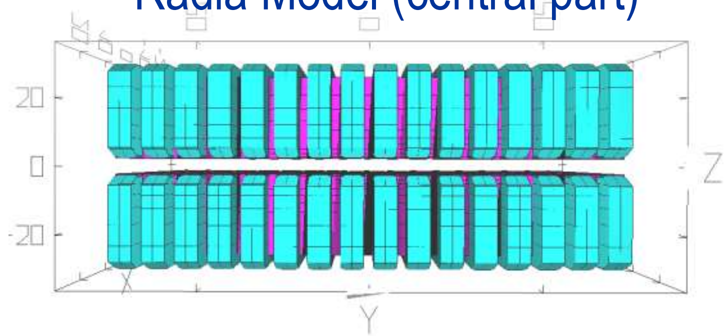
M. Rakitin (NSLS-II)
D. Bruhwiler, R. Nagler, P. Moeller, B. Nash

radiasoft

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

Radia Model (central part)



IVU Parameters

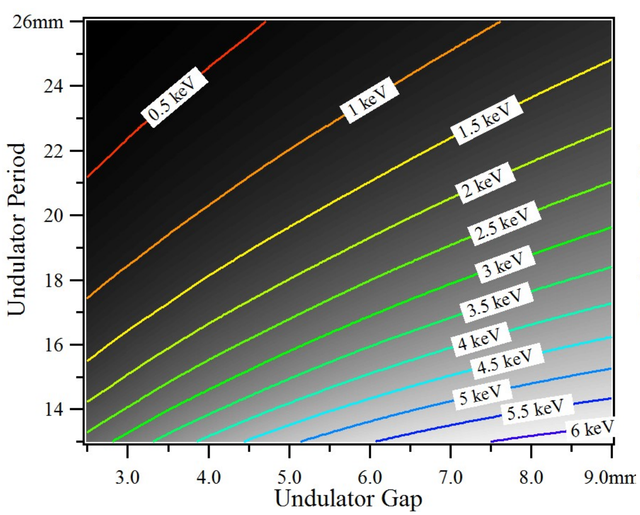
Reference Geometry:

- 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

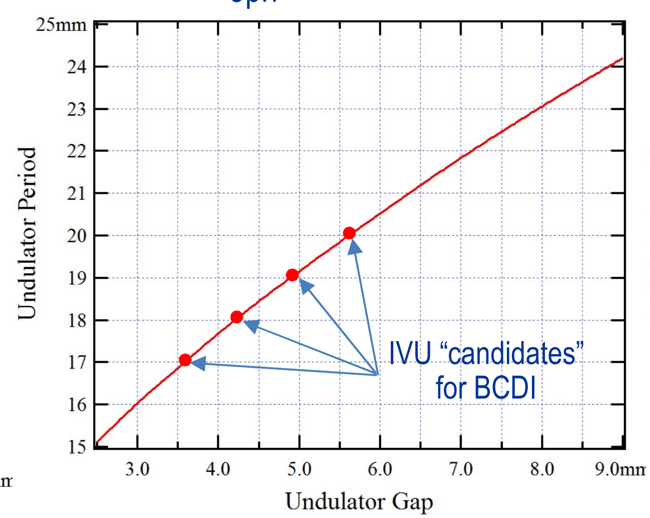
Materials:

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

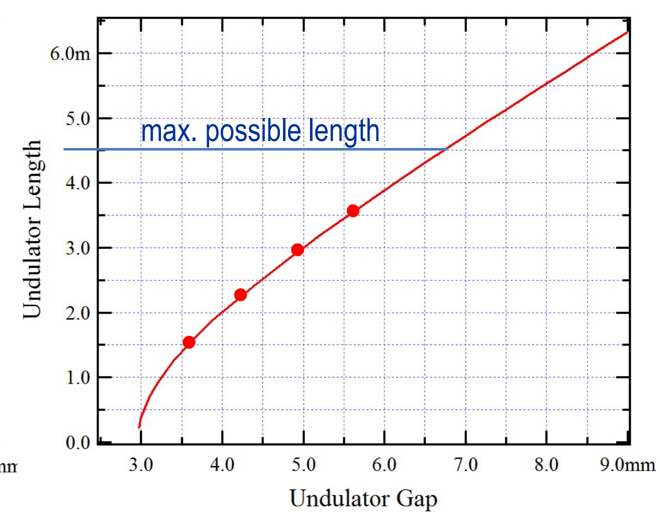
Fundamental Photon Energy vs IVU Gap and Period at E_{el} = 3 GeV



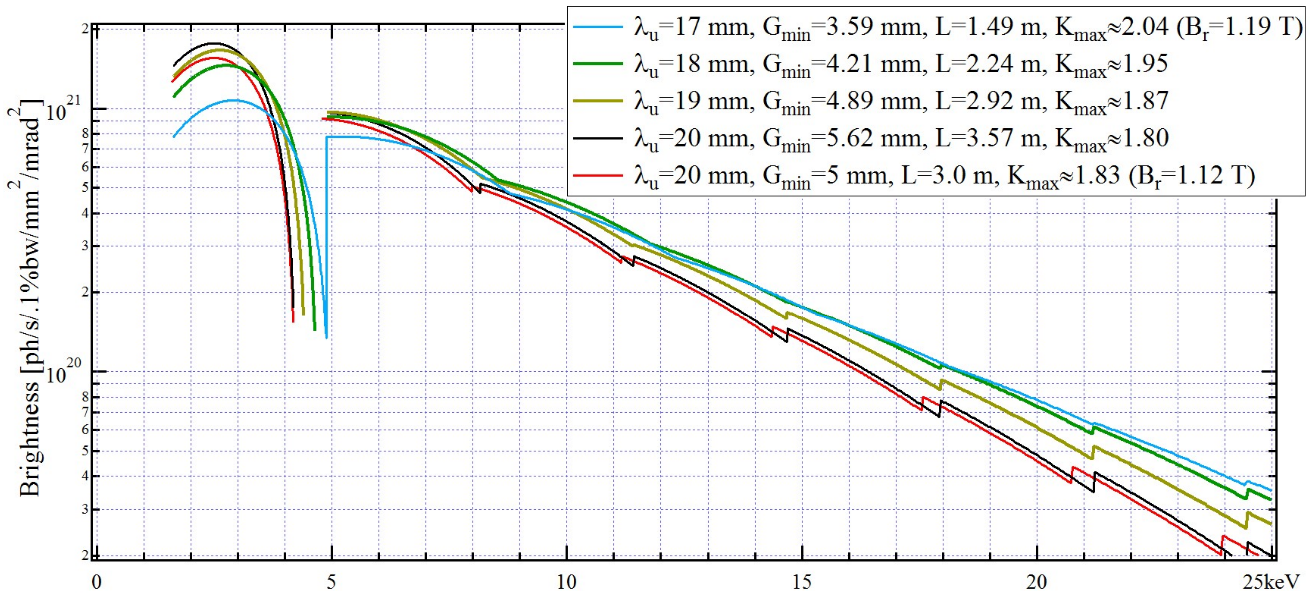
IVU Period vs Gap at E_{1ph} = 1.633 keV ($E_{3ph} \approx$ 4.9 keV)

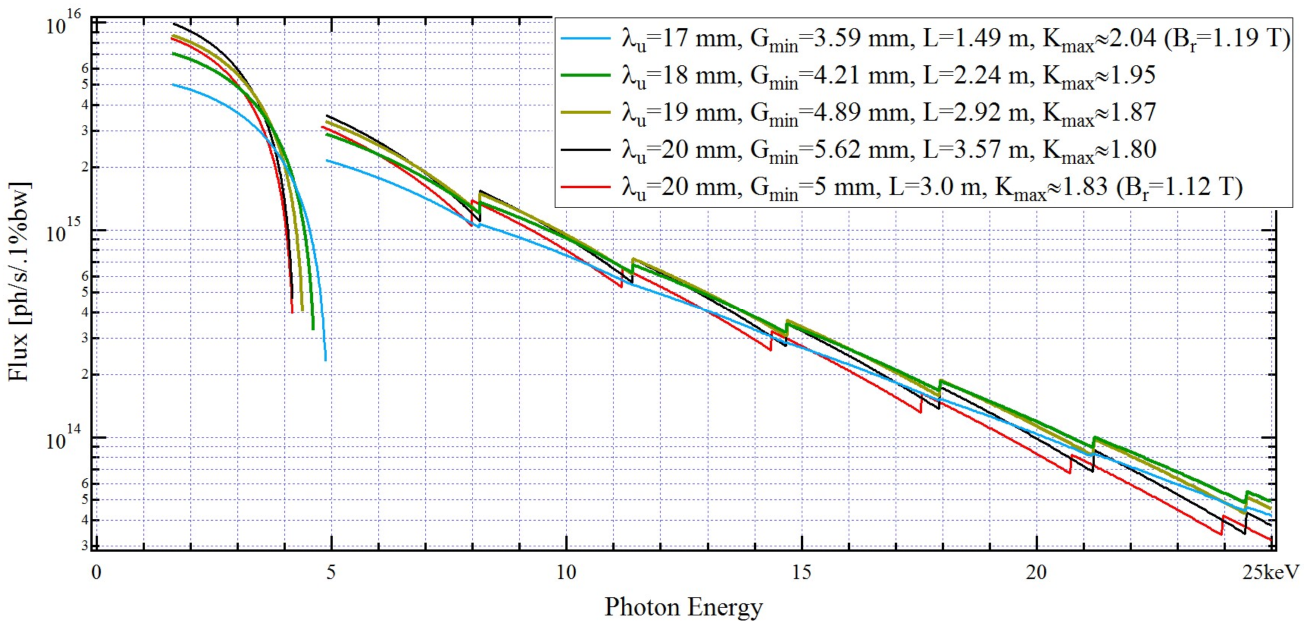


Maximal IVU Length vs Gap for Low-Beta Straight Section of NSLS-II (geom. "stay clear")



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



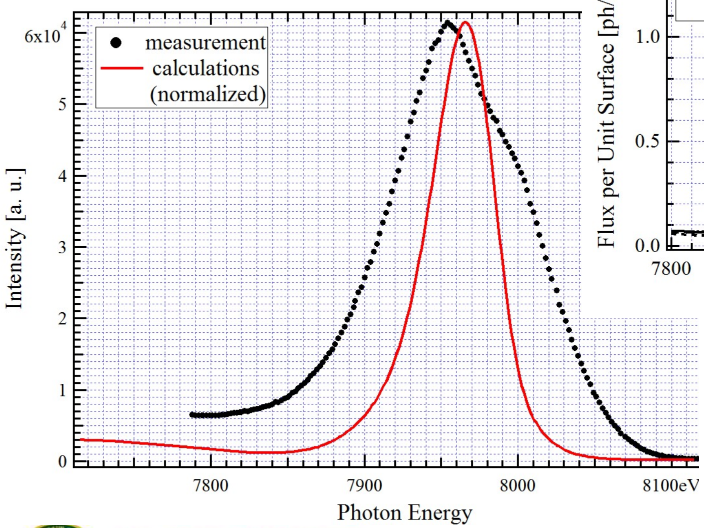


ε_x = 0.9 nm
β_{x0} = 1.84 m
ε_y = 8 pm
β_{y0} = 1.17 m

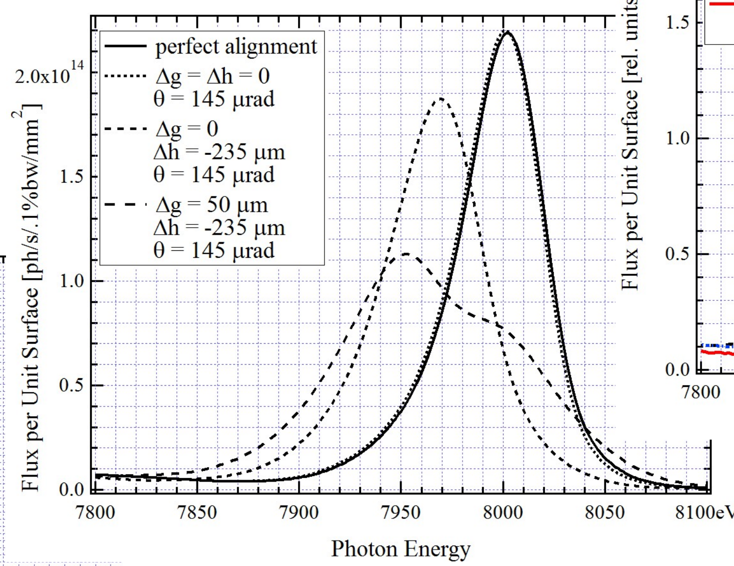
Spectrum-Based Alignment of IVU21 with Respect to Electron Beam at SRX Beamline of NSLS-II

Initial On-Axis Spectrum Measured at 5th UR Harm. at ~6.8 mm Gap Compared to the Corresponding Calculated Spectrum

The calculation was based on measured magnetic field; two spectra are normalized to same max. value.

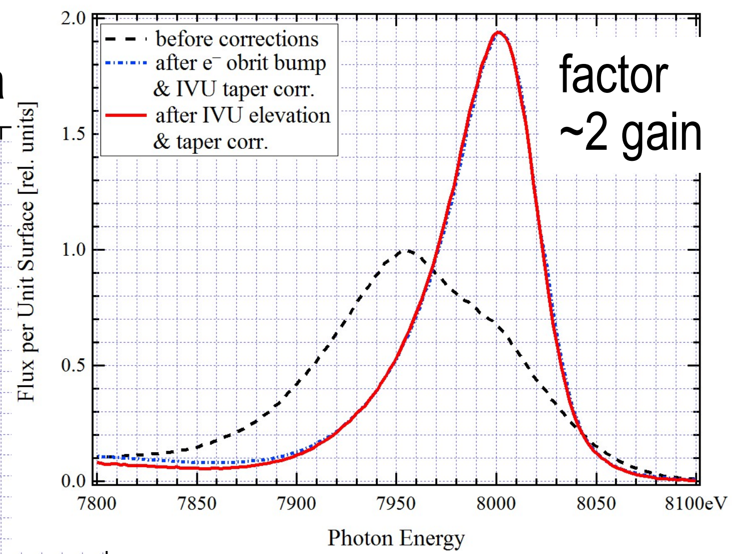


SRW Simulation of IVU Misalignment Effects – "Gap Taper" and "Tilt of Magnet Arrays + Elevation" – on the On-Axis UR Spectral Flux per Unit Surface Area



Parametric dependencies of the IVU misalignment effects on magnetic field were determined from magnetic simulations with Radia code and from magnetic measurements.

Measured On-Axis Spectral Flux per Units Surface Area Before and After the Spectrum-Based IVU Alignment

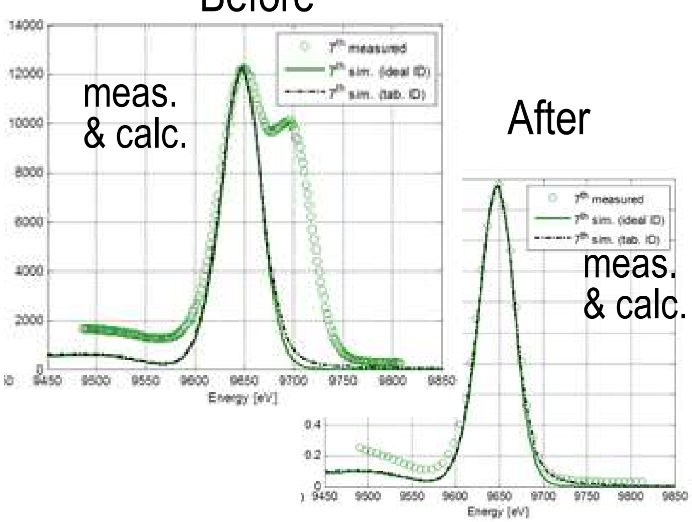


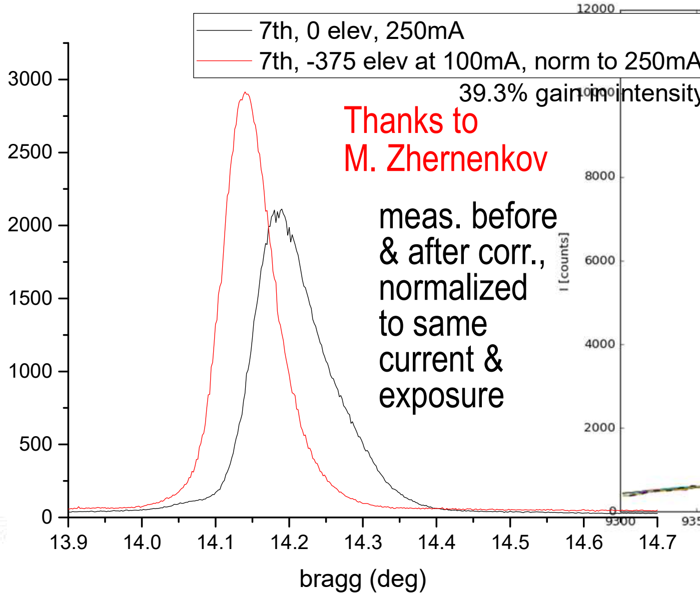
The best spectral performance was reached by modifying the IVU gap taper (gap diff. bw exit and entrance) by $\Delta g \approx 50$ µm and changing the elevation by $\Delta h \approx 250$ µm, in agreement with simulation predictions.

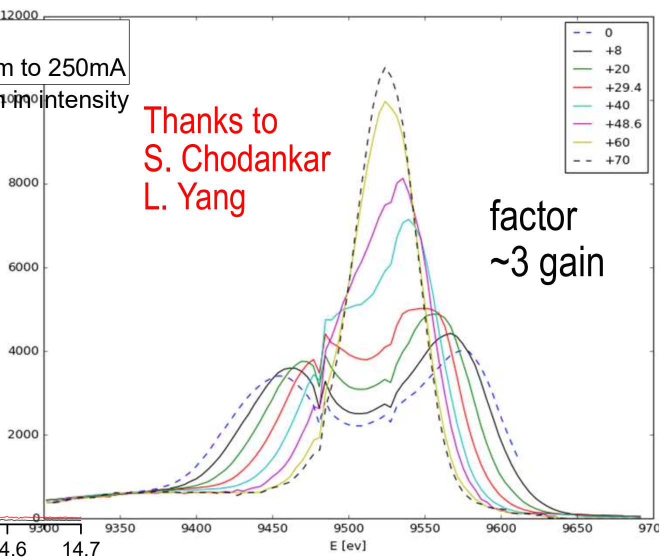
Spectrum Based Alignment of IVUs at Other Hard X-ray Beamlines of NSLS-II

On-Axis UR Spectra Before and After Spectrum Based Alignment

IVU20 - 3 m at **CHX**	IVU23 - 2.8 m at **SMI**	IVU23 - 2.8 m at **LiX**
(harm. #7 at ~5.2 mm gap, ~9.65 keV)	(harm. #7 at ~6.5 mm gap, ~8.07 keV)	(harm. #9 at ~6.2 mm gap, ~9.24 keV)







Spectral performance was fully restored by introducing ~300 μm change in IVU elevation.

Spectral performance was ~fully restored by introducing -400 μm change in elevation (the IVU was re-aligned mechanically then).

Spectral performance was restored by introducing ~70 μm change in taper.

Spectral performance of ~One Half of NSLS-II IVUs was restored / improved thanks to the Spectrum-Based Alignment

Decisive contributions by D. Hidas (advanced IVU control)

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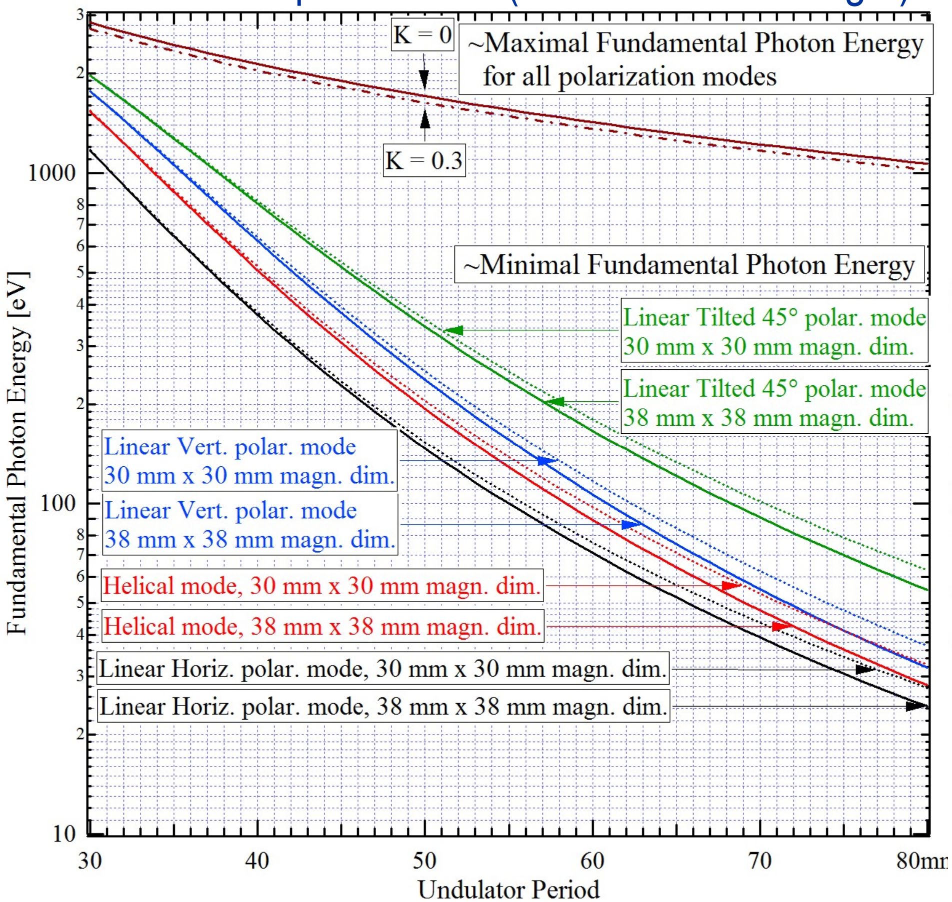
APPLE-II Elliptically-Polarizing Undulator (EPU) Period Choice at NSLS-II

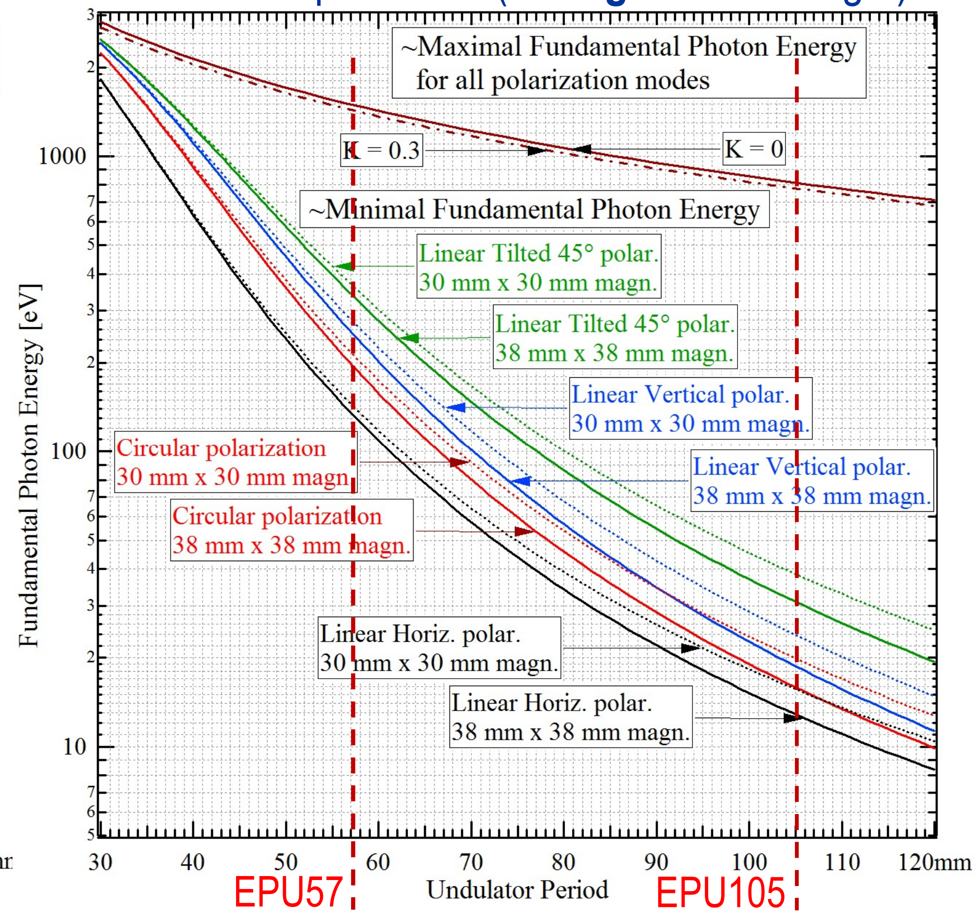
Minimal and Maximal Photon Energies of the Fundamental vs Undulator Period for E = 3 GeV

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

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



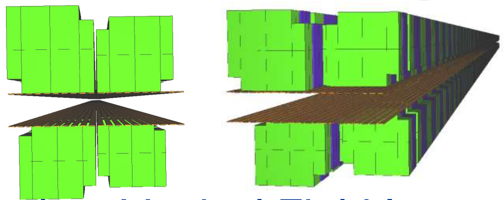
Minimal Gap: **16 mm** (for **High-Beta** Straight)



APPLE-II structure was invented by S. Sasaki

RADIA simulations

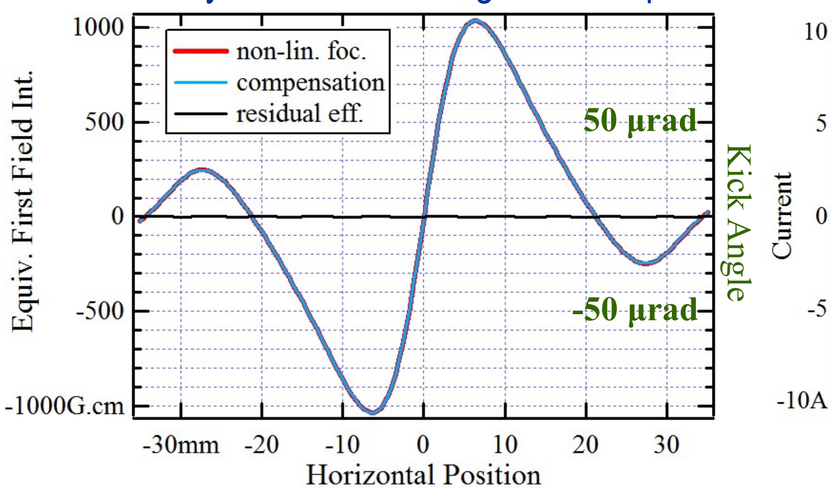
Compensation of EPU105 Nonlinear Focusing Effects by Current Strips in Linear Vertical Polarization Mode at 19 mm Gap ($E_{ph\ min} \approx 30$ eV)

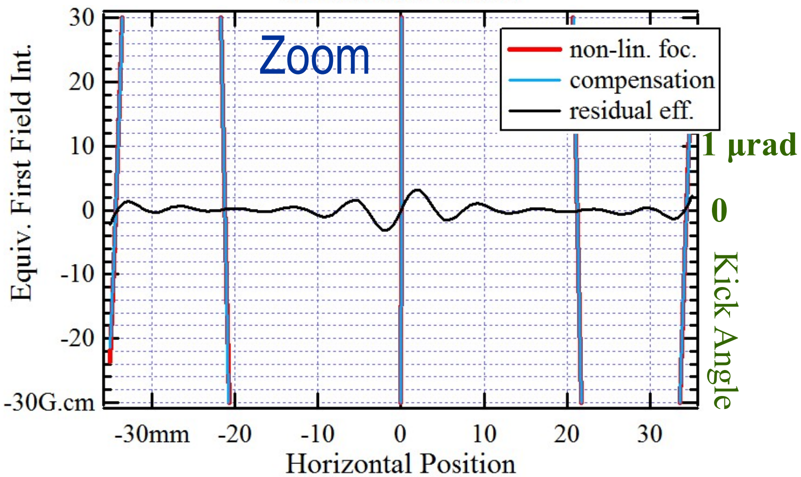


Current Strips Idea: I. Blomqvist

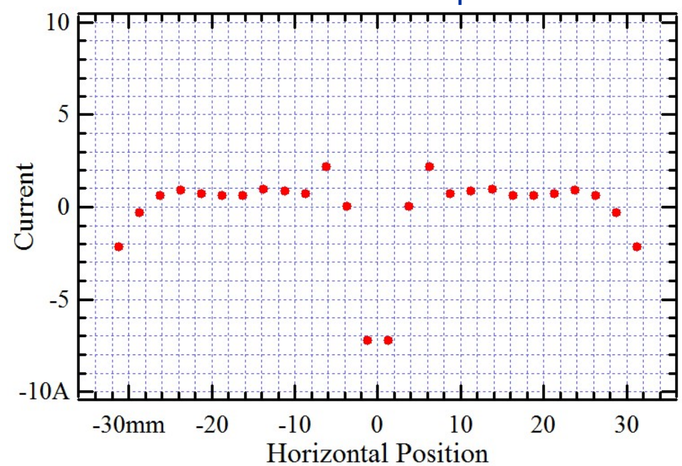
First Implementation: J. Bahrdt (BESSY)

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):

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

Tikhonov Matrix

In these calculations, it was used:

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

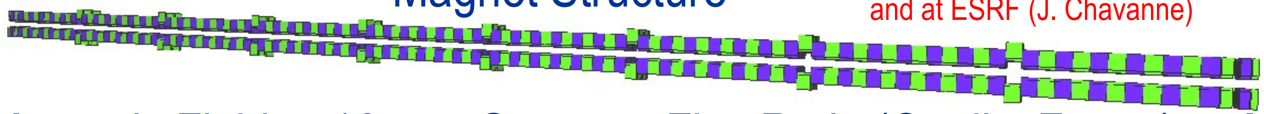
Regularization Parameter allowing to control norm of solution (i.e. max. currents)

Unit Matrix

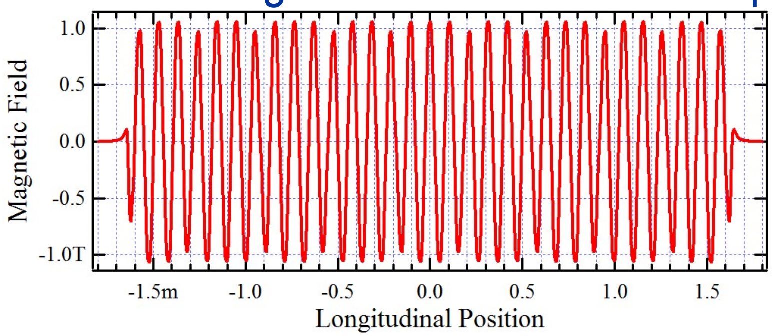
EPU105 Quasi-Periodic Option

Magnet Structure

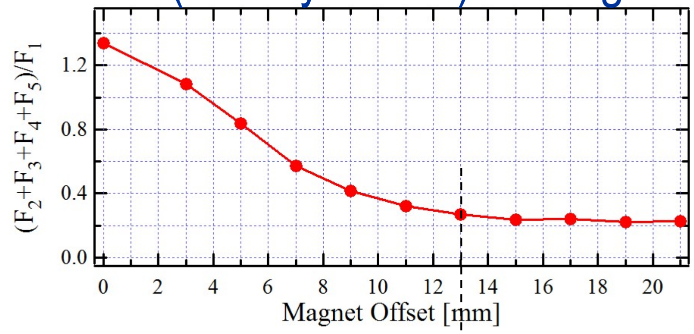
This / similar method was first used at ELETTRA (B. Diviacco) and at ESRF (J. Chavanne)



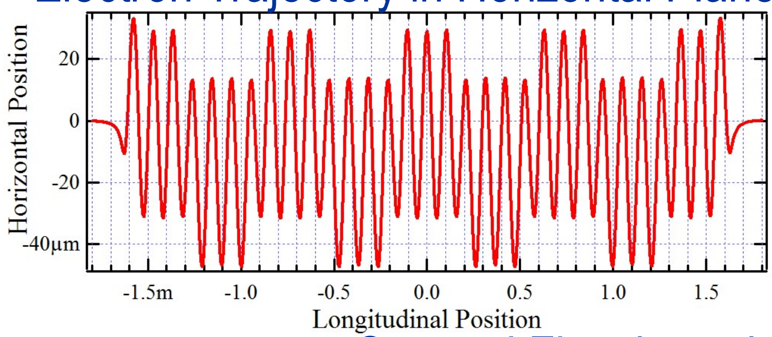
Vertical Magnetic Field at 16 mm Gap



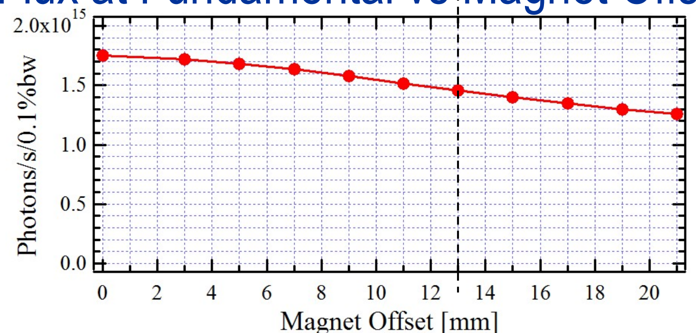
Flux Ratio (Quality Factor) vs Magnet Offset



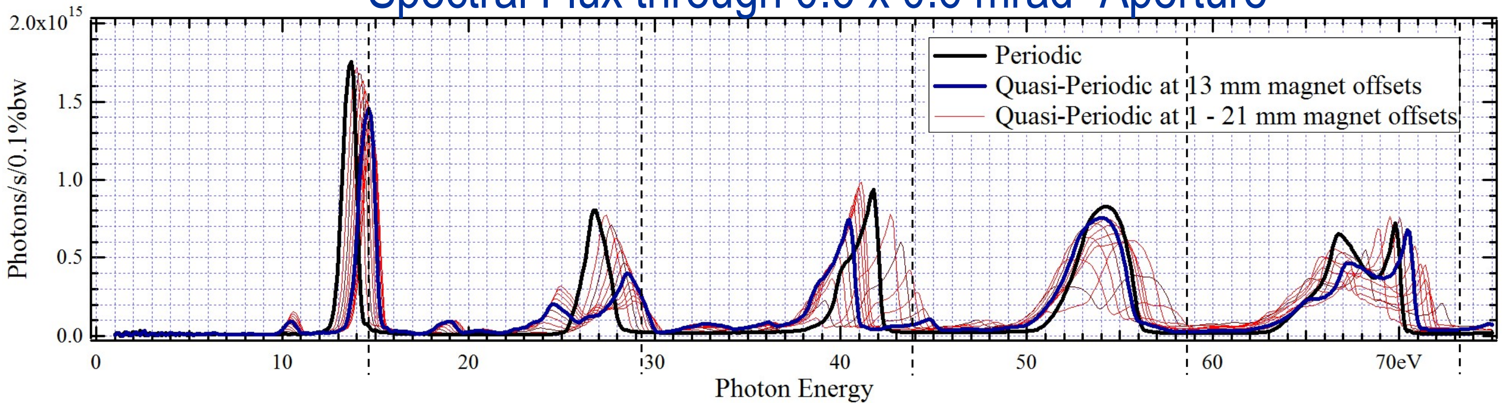
Electron Trajectory in Horizontal Plane



Flux at Fundamental vs Magnet Offset



Spectral Flux through 0.6 x 0.6 mrad^2 Aperture

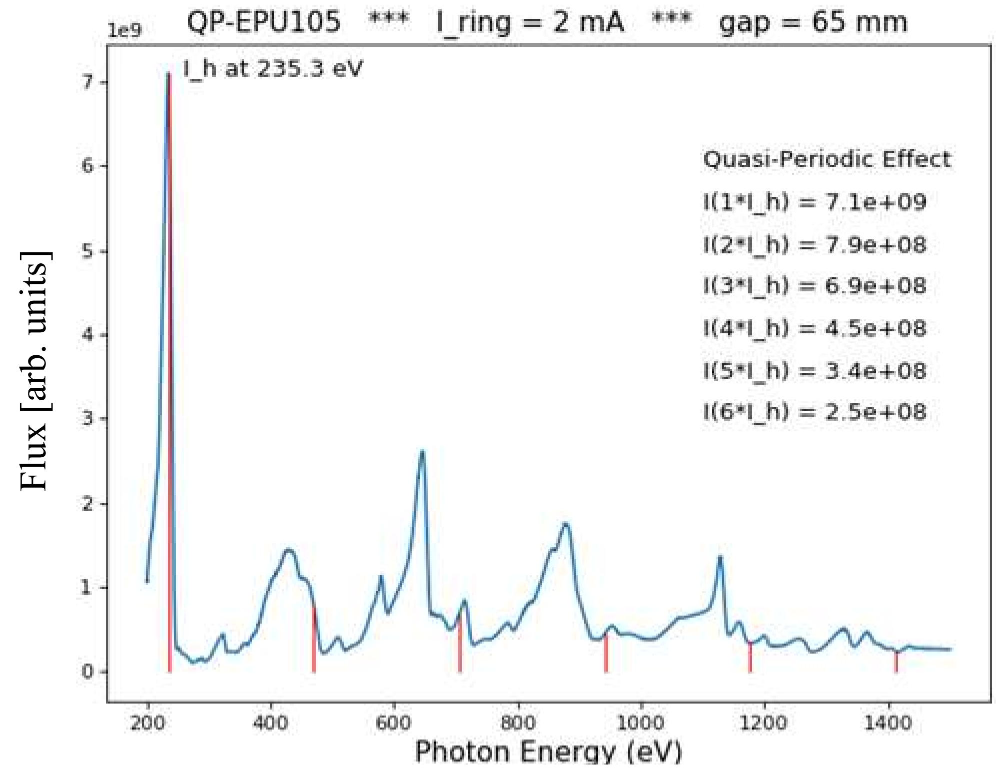


EPU105 was magnetically assembled and shimmed in-house at NSLS-II using IDBuilder code.

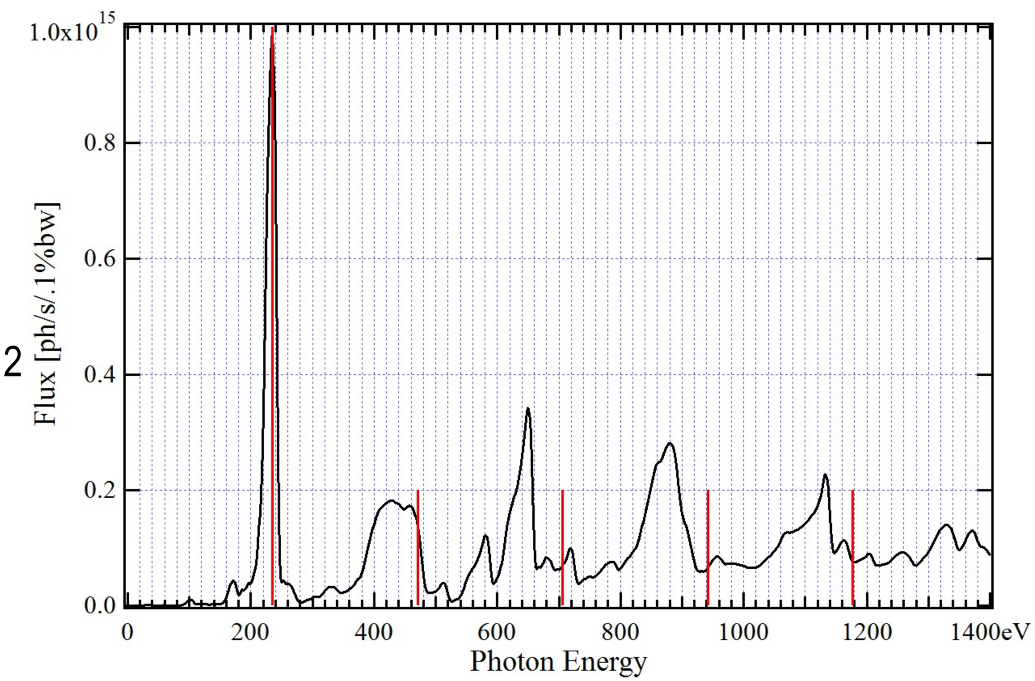
C. Kitegi
M. Musardo

EPU105 Quasi-Periodic Spectrum
at 65 mm Gap

Measured at ESM
normalized by estimated detector response



Calculated
based on measured **B**(z)
aperture: 0.16 x0.16 mrad^2



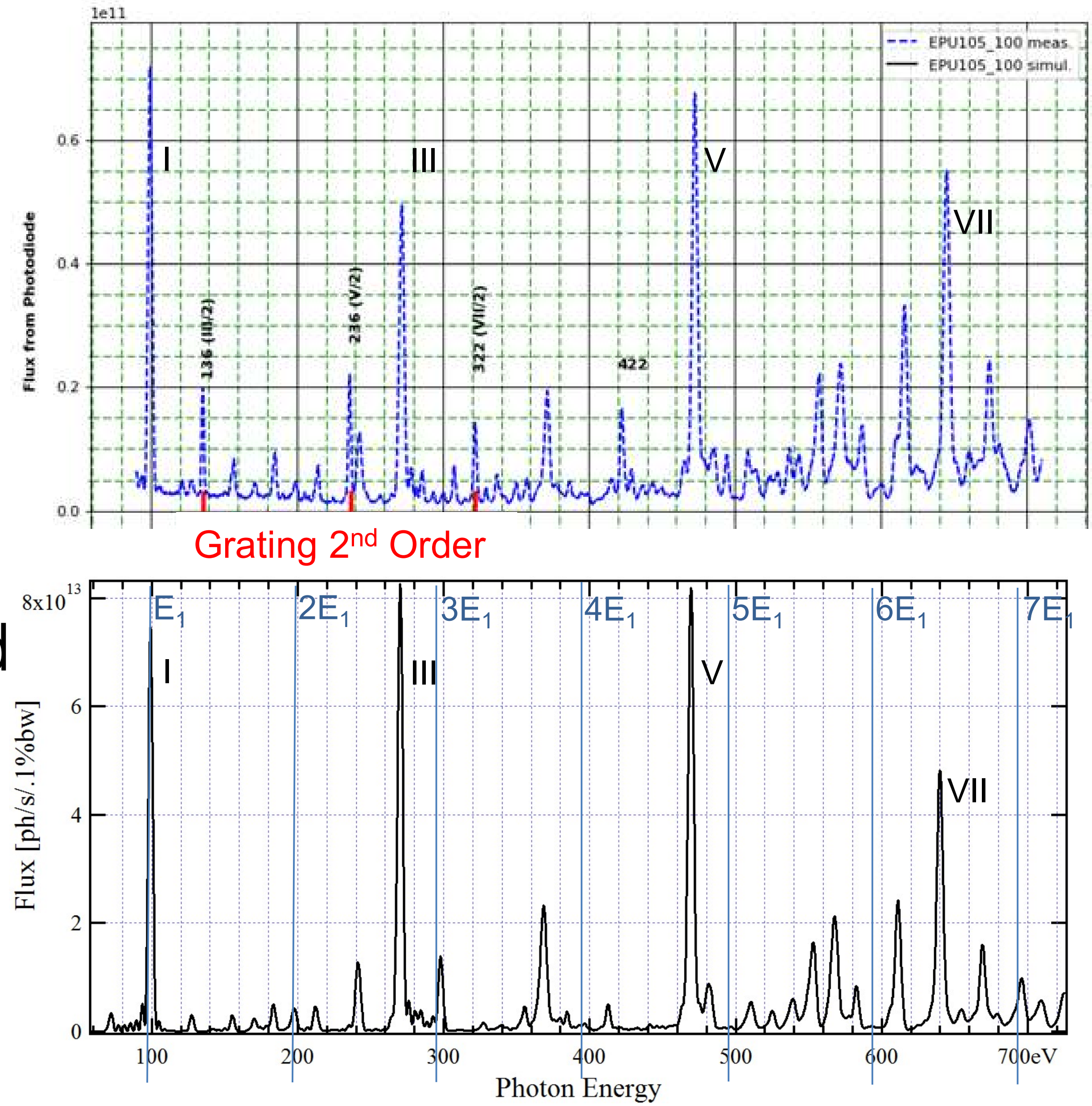
EPU105 Quasi-Periodic Spectrum

at 48 mm Gap

E. Vescovo

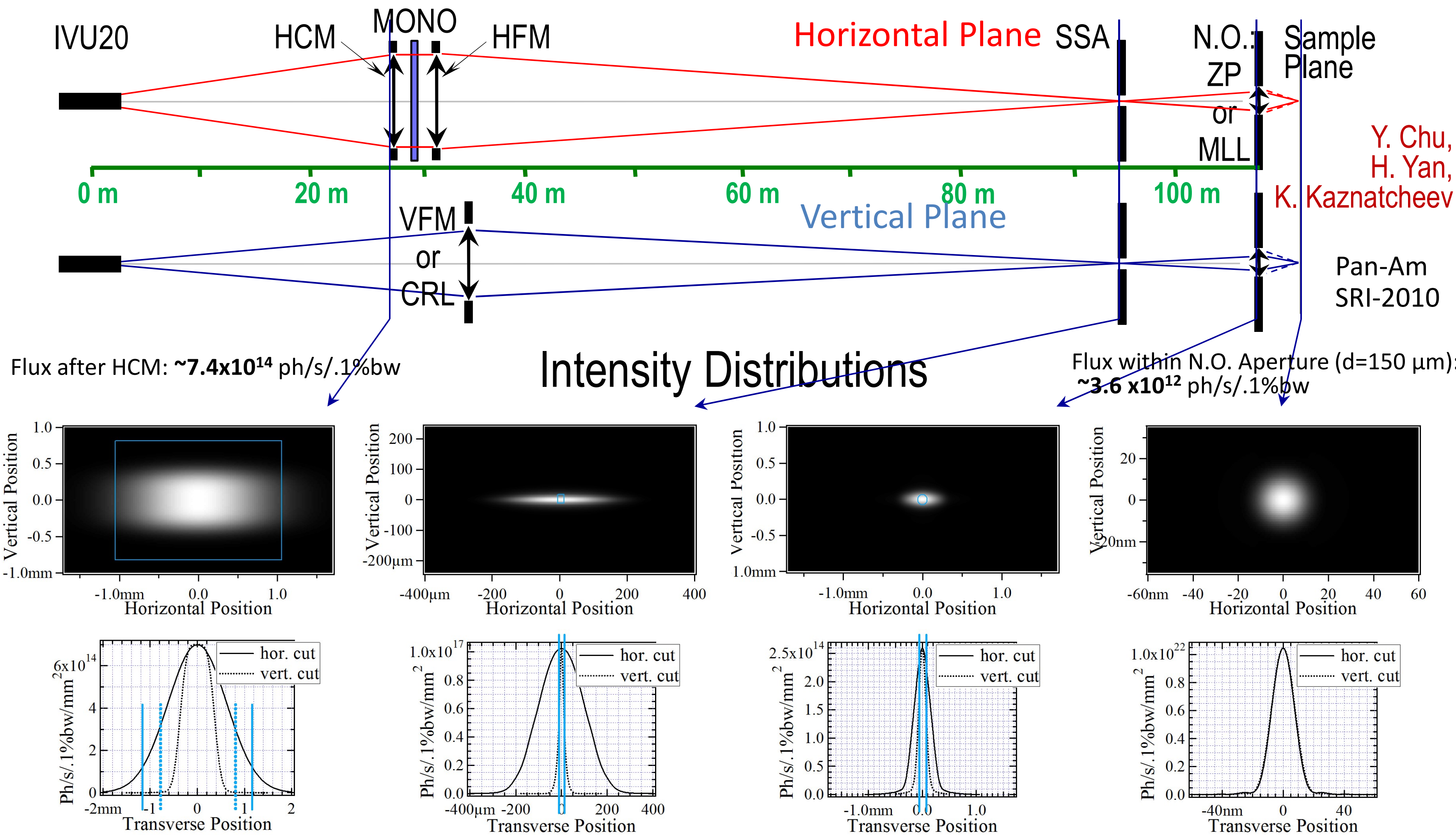
Measured at ESM

Calculated based on measured **B**(z)

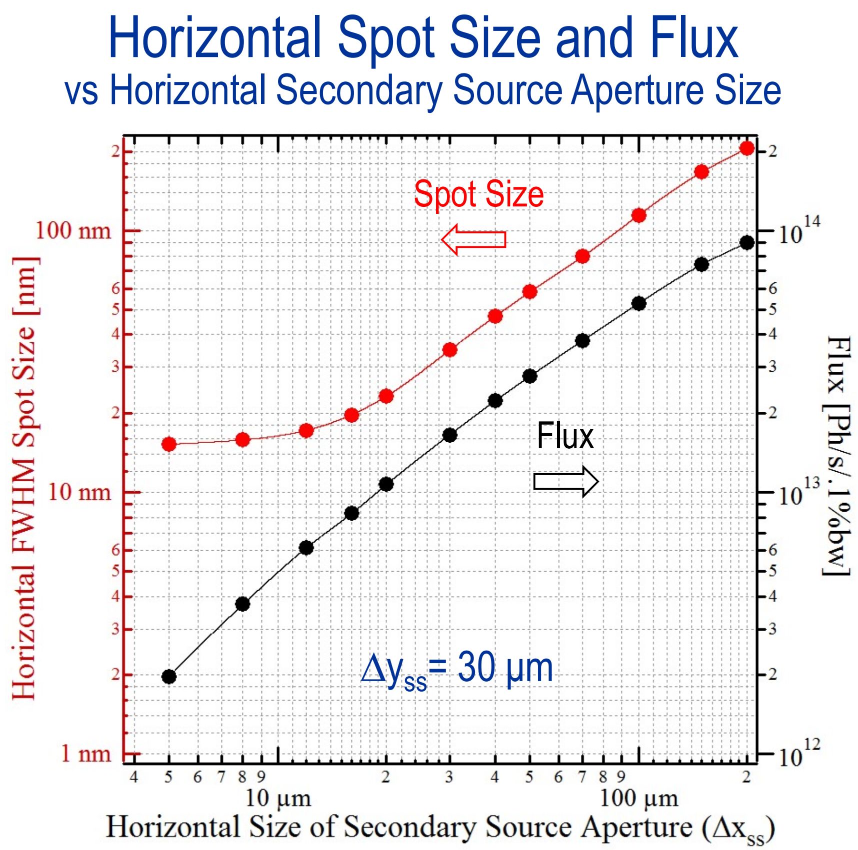


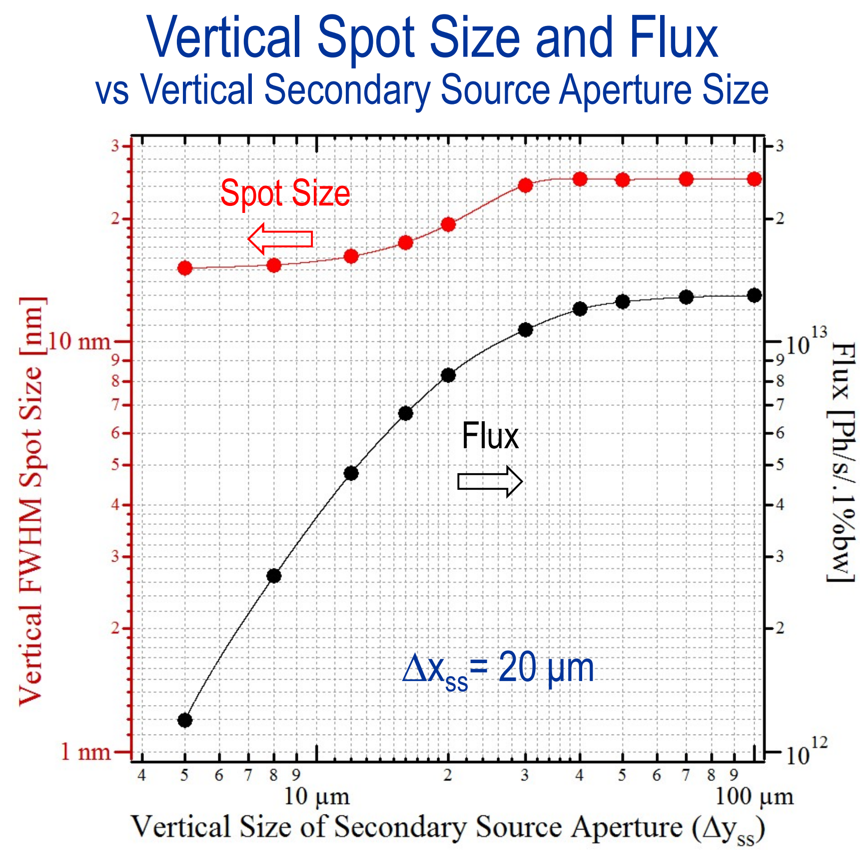
Quasi-Periodic Undulator does its job: grating's 2nd order peaks are shifted off UR harmonics

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



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





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)

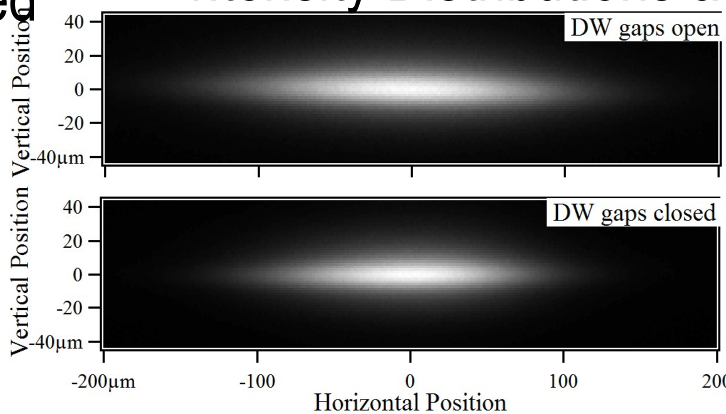
Electron Beam Imaging Near Secondary Source Aperture (at ~63 m from undulator) of HXN Beamline

Intensity Distributions at 8.0 keV (5th UR harmonic)

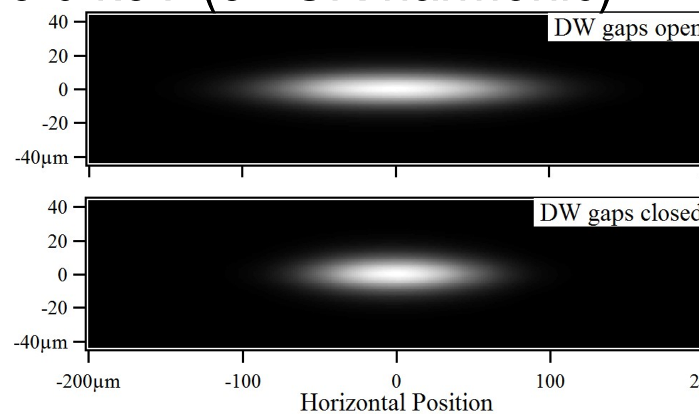
Measured

DW Gaps Open

DW Gaps Closed



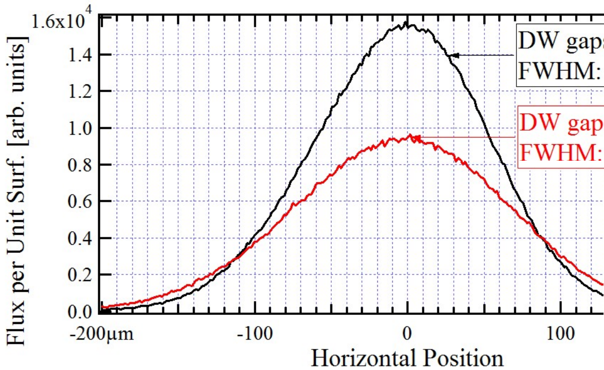
Calculated

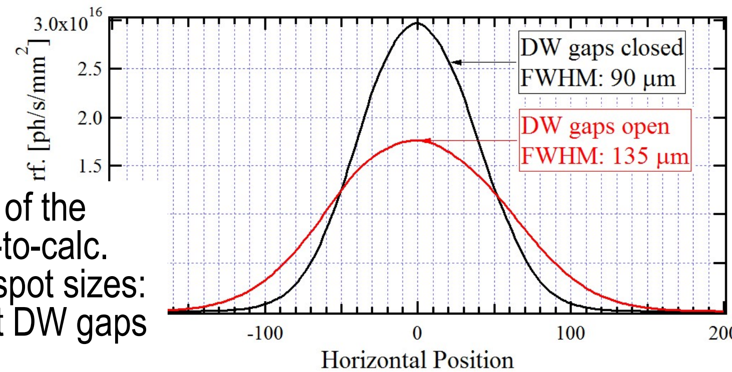


DW gaps open: $\varepsilon_x \approx 2.1$ nm, $\sigma_{ex} \approx 61$ µm

DW gaps closed: $\varepsilon_x \approx 0.9$ nm, $\sigma_{ex} \approx 40$ µm

Cuts by Horizontal Mid-Plane





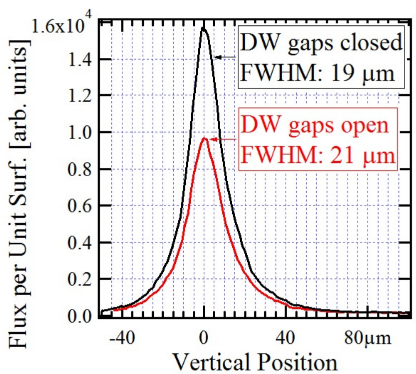
Optical magn. ~0.93

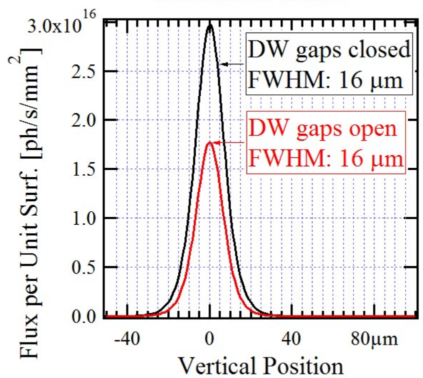
Assumption of error-free optical elements

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

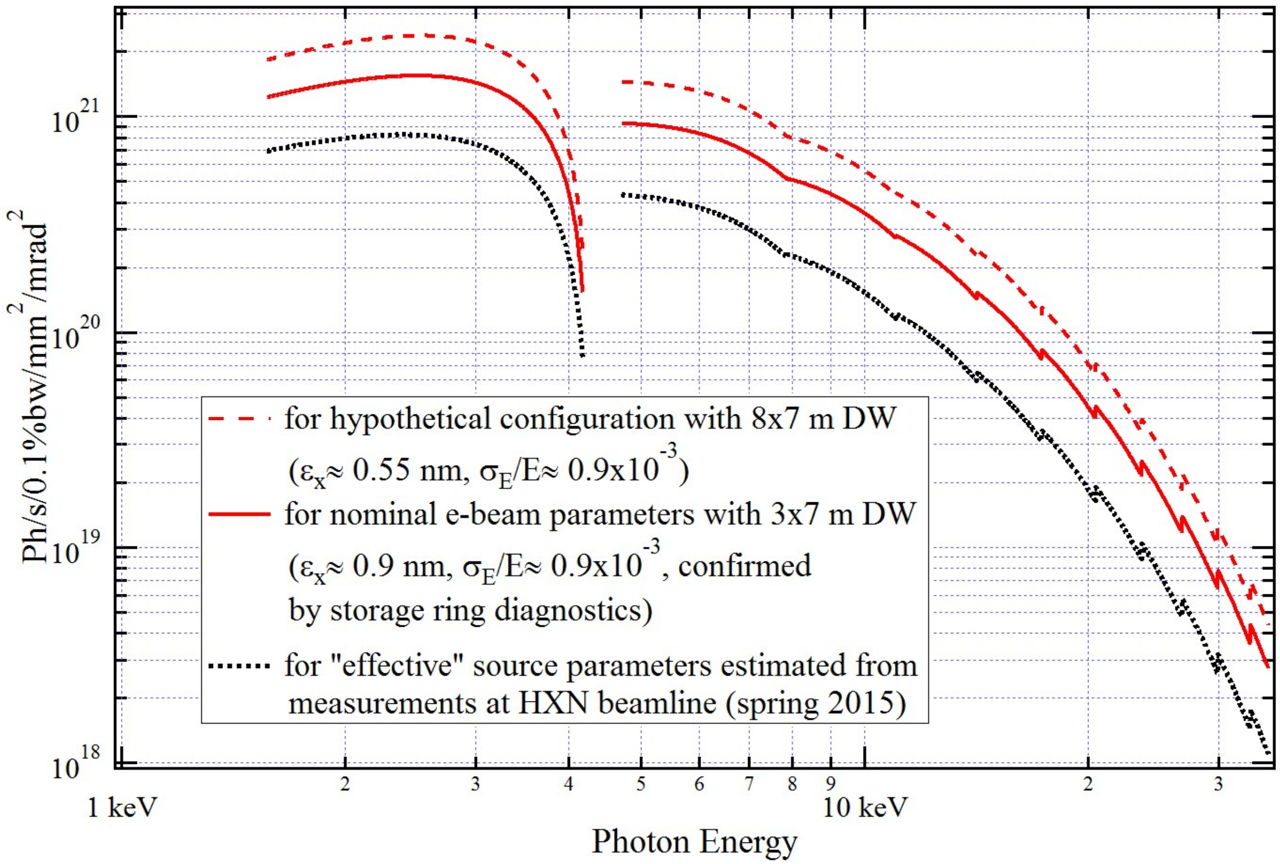




$\varepsilon_y \approx 30$ pm
$\sigma_{ey} \approx 5.9$ µm

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.

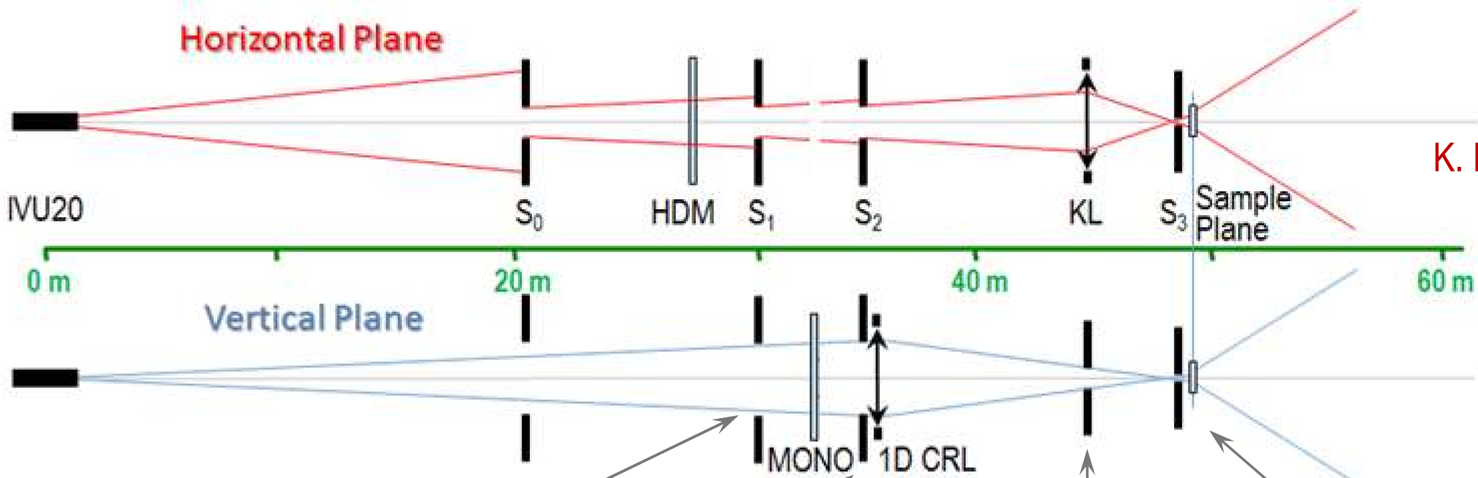
Note: absolute values of spectral brightness may not be very accurate, however, relative "locations" of the curves are credible.

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



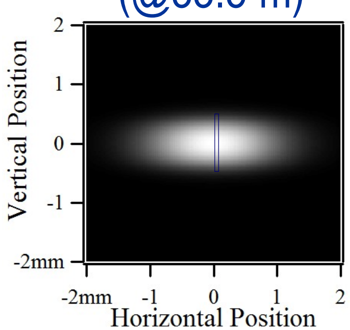
Intensity Distributions

for E = 10 keV

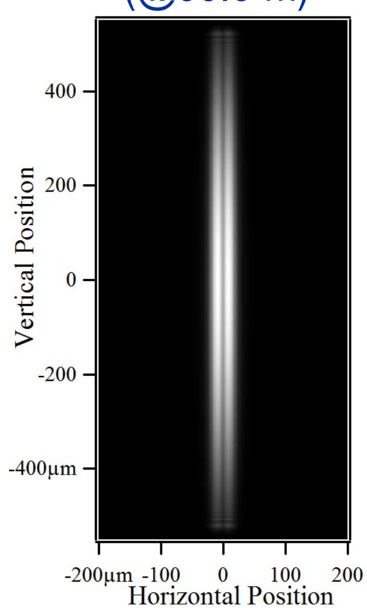
ΔS_{1x}= 44 μm

ΔS_{1y}= 1 mm

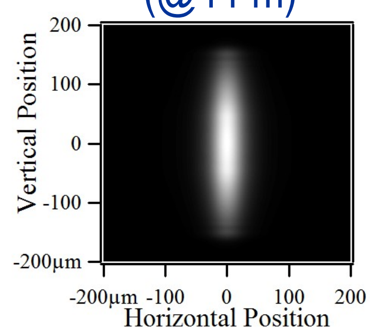
Before SS1
(@33.5 m)



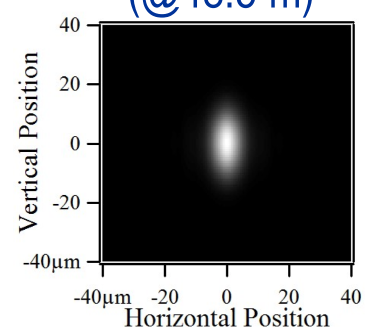
Before CRL
(@35.8 m)



Before KL
(@44 m)



At Sample
(@48.5 m)



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

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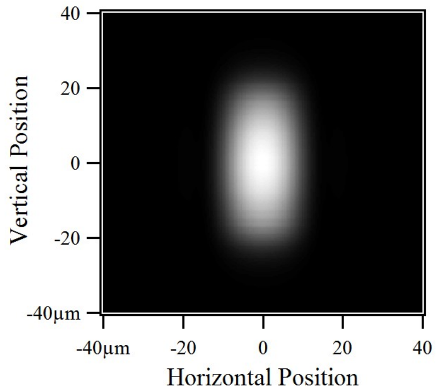
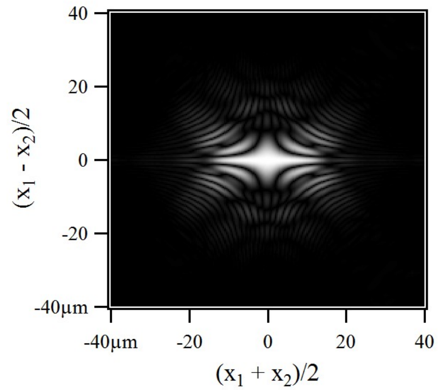
Tracking Intensity and Degree of Transverse Coherence at CHX Sample

Intensity Distribution

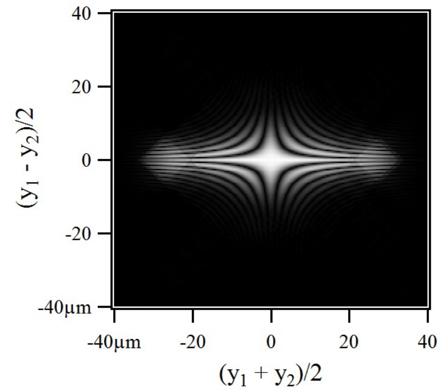


Degree of Transverse Coherence

In Horizontal Mid-Plane

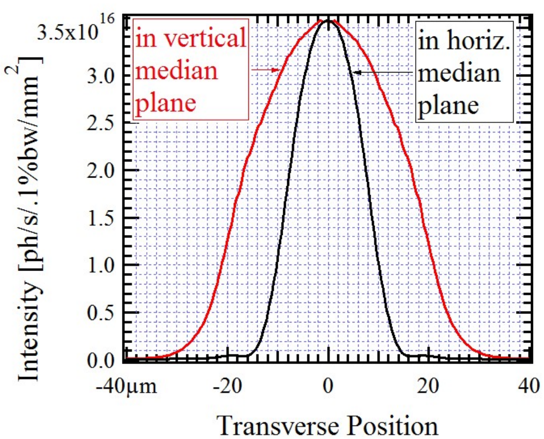


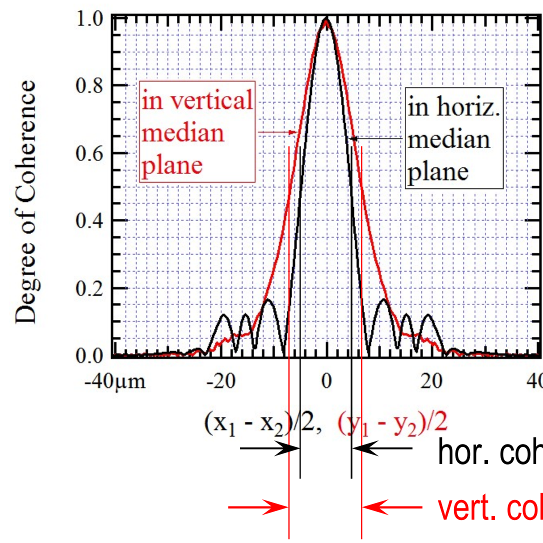
In Vertical Mid-Plane



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

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



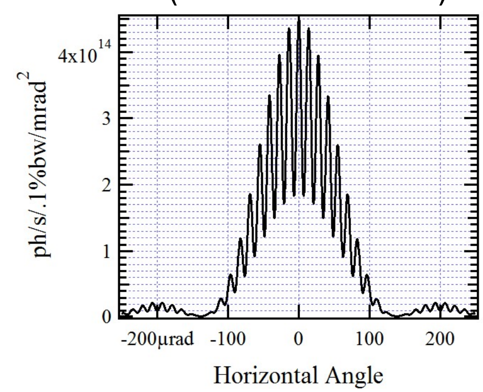


hor. coherence length: ~9.4 µm

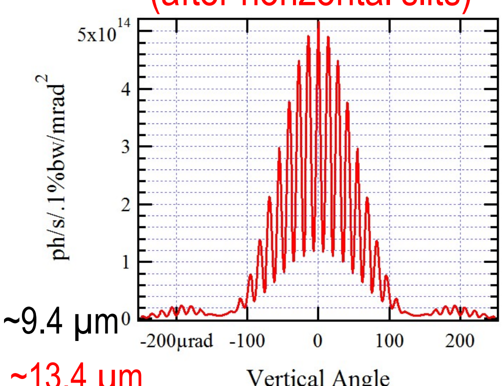
vert. coherence length: ~13.4 µm

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

In Horizontal Plane (after vertical slits)



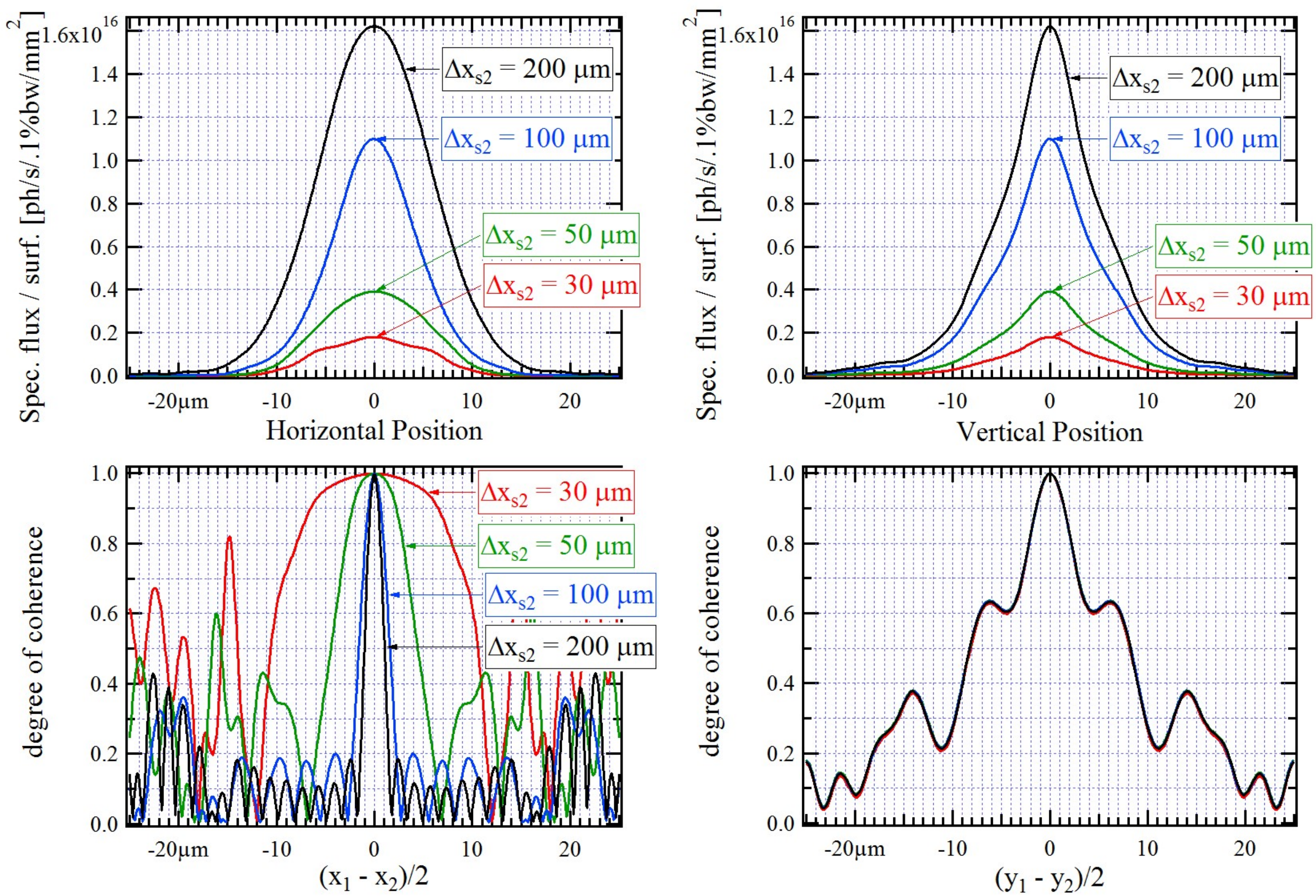
In Vertical Plane (after horizontal slits)



Good agreement with 2-slit interference simulation results

Simulation of Coherent Scattering Experiments (CHX):

Horizontal and Vertical Mid-Plane Cuts of Intensity Distributions and Degree of Coherence at Sample

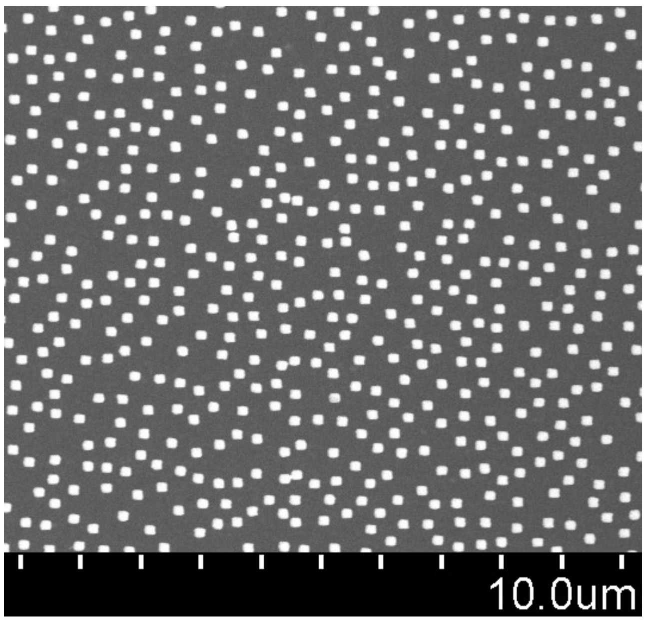


FWHM size of central lobe of a Degree of Coherence curve gives horizontal (vertical) Coherence Length.
The horizontal Coherence Length varies from ~2.1 µm (at Δx_{S2}= 200 µm) to ~20 µm (at Δx_{S2}= 30 µm).
The horizontal FWHM (intensity) spot size is ~10 µm in all cases.
The vertical coherence length is ~16 µm and spot size ~9.7 µm in all cases.

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

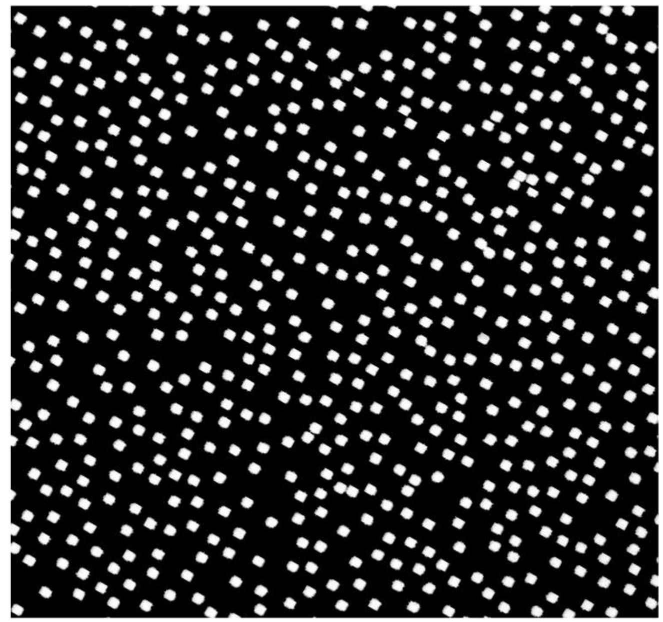
M. Rakitin

Original EM 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 Image

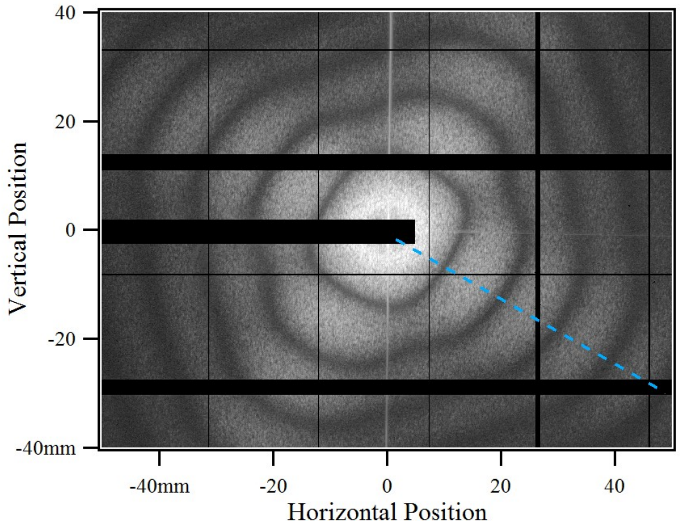


Processed and rotated image was used as input for definition of a Transmission object for SRW simulation. Rotation was added to simulate sample orientation used in the actual experiment.

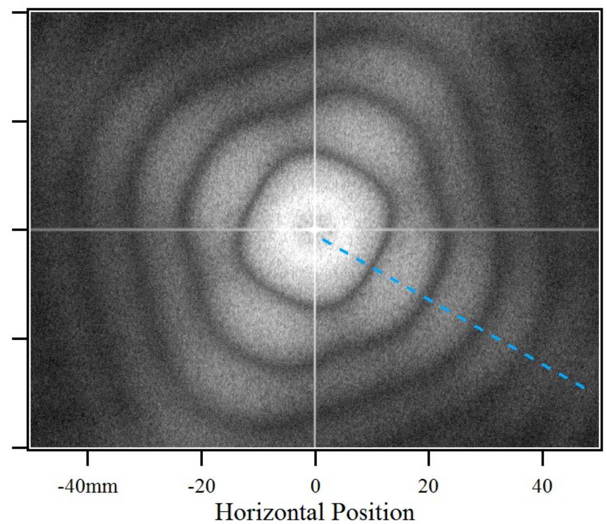
Simulation of Coherent Scattering Experiments (CHX):

Speckle Patterns

Measured



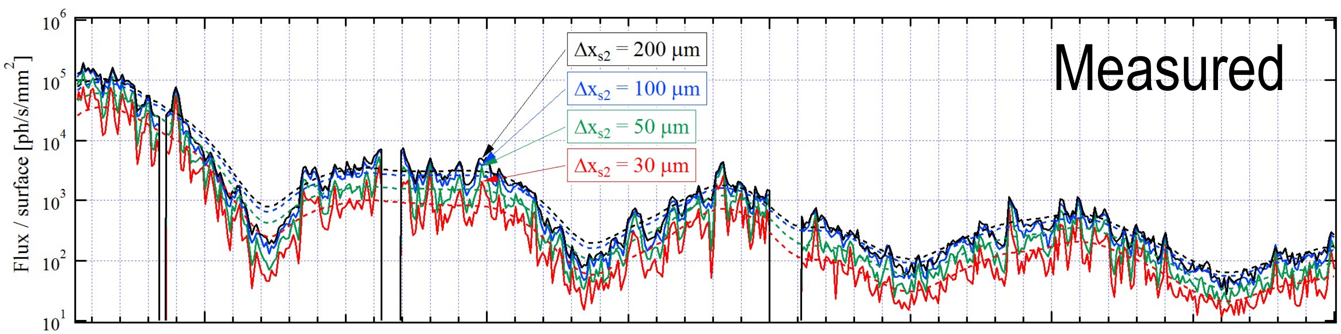
Simulated

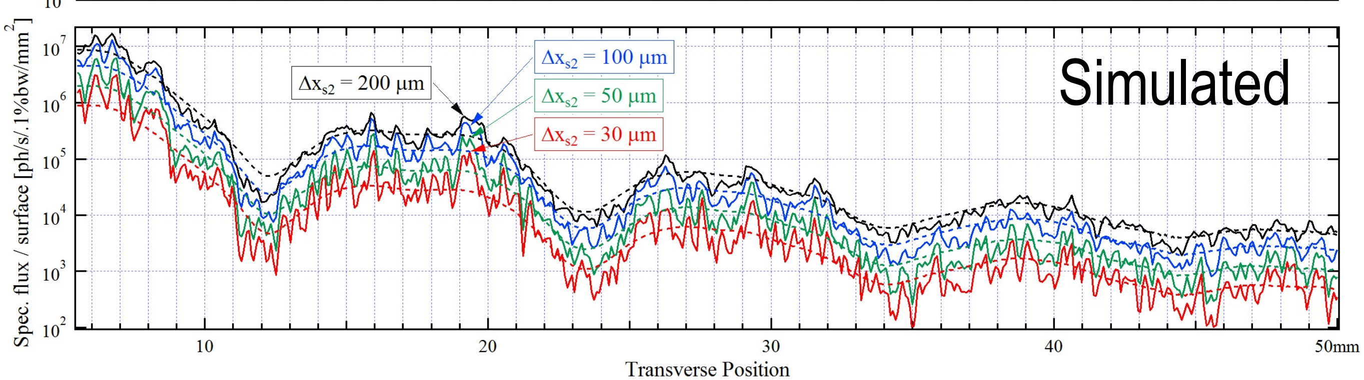


E_{ph} = 9.65 keV

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
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Summary

- **High-accuracy calculations** in the areas of **magnet design**, **synchrotron emission** and **propagation** through beamline optics, and **interaction of the radiation with samples** in some experiments, **can be done** for current and future light sources, using the **existing computer codes**.
- These calculations facilitate a **balanced**, **well-matched approach to development of new light sources**, which brings insertion devices, X-ray optics, and experimental setups in agreement with properties of the emitting electron beam.

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