Fourier-Optics Compatible Radiation Propagation Methods Used in SRW

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Wavefront Propagation in the Case of Full Transverse Coherence

Kirchhoff Integral Theorem applied to Spontaneous Emission by One Electron

\[ \mathbf{E}_{\omega 2\perp} (P_2) \approx \frac{k^2 e^{i\omega t}}{4\pi} \int_0^\infty \int_A \mathbf{B}_{\omega 1\perp} - \mathbf{n}_\perp \exp [i(k(c\tau + R + S)) \cdot (\ell \cdot \mathbf{n}_{p_1p_2} + \ell \cdot \mathbf{n}_{p_1p_2})] d\Sigma \]

Valid at large observation angles; Is applicable to complicated cases of diffraction inside vacuum chamber

Huygens-Fresnel Principle

Fourier Optics

Free Space: (between parallel planes perpendicular to optical axis)

\[ \mathbf{E}_{\omega 2\perp}(x_2, y_2) \approx \frac{k}{2\pi iL} \int \mathbf{E}_{\omega 1\perp}(x_1, y_1) \exp [i(kL^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2)] dx_1 dy_1 \]

Assumption of small angles

"Thin" Optical Element:

\[ \mathbf{E}_{\omega 2\perp}(x, y) \approx \mathbf{T}(x, y, \omega) \mathbf{E}_{\omega 1\perp}(x, y) \]

"Thick" Optical Element: (propagation from transverse plane before the element to a transverse plane just after it)

\[ \mathbf{E}_{\omega 2\perp}(x_2, y_2) \approx \mathbf{G}(x_2, y_2, \omega) \exp [ik \Lambda(x_2, y_2, k)] \mathbf{E}_{\omega 1\perp}(x_1(x_2, y_2), y_1(x_2, y_2)) \]

Implemented in SRW for Python in 2012; Currently used for simulation of NSLS-II PX and spectral microscopy beamlines

Benchmarking against experimental data is required
Approach to High-Accuracy Partially-Coherent Emission and Wavefront Propagation Simulations

Averaging (over phase-space volume occupied by e-beam) of the intensity (or mutual intensity, or mathematical brightness) obtained from electric field emitted by an electron and propagated through an optical system:

\[ I_\omega (x, y) = \int I_{\omega1} (x, y; x_e, y_e, z_e, x'_e, y'_e, \delta y_e) f(x_e, y_e, z_e, x'_e, y'_e, \delta y_e) \, dx_e \, dy_e \, dz_e \, dx'_e \, dy'_e \, d\delta y_e \]

\[ I_{\omega1} (x, y; x_e, y_e, z_e, x'_e, y'_e, \delta y_e) = |E_{\omega1} (x, y; x_e, y_e, z_e, x'_e, y'_e, \delta y_e)|^2 \]

\[ M_{\omega1} (x, y, \tilde{x}, \tilde{y}; x_e, y_e, z_e, x'_e, y'_e, \delta y_e) = E_{\omega1} (x, y; x_e, y_e, z_e, x'_e, y'_e, \delta y_e) E_{\omega1}^* (\tilde{x}, \tilde{y}; x_e, y_e, z_e, x'_e, y'_e, \delta y_e) \]

\[ B_{\omega1} (x, y, \theta_x, \theta_y; x_e, y_e, z_e, x'_e, y'_e, \delta y_e) = E_{\omega1} (x, y; x_e, y_e, z_e, x'_e, y'_e, \delta y_e) \int E_{\omega1} (\tilde{x}, \tilde{y}; x_e, y_e, z_e, x'_e, y'_e, \delta y_e) \exp \left[ i \frac{\omega}{c} (\theta_x \tilde{x} + \theta_y \tilde{y}) \right] d\tilde{x} d\tilde{y} \]

This method is general and accurate. For the most part, it is already implemented in SRW code. However, it can be CPU-intensive, requiring parallel calculations on a multi-core server or a small cluster. Several approaches are considered for increasing the efficiency, including use of low-discrepancy sequences (collaboration with R. Lindberg, K.-J. Kim, X. Shi, ANL), “improved Monte-Carlo” type techniques, as well as “coherent mode decomposition”.

NOTE: the smaller the e-beam emittance (the higher the radiation coherence) – the faster is the convergence of simulations with this general method.

NOTE: convolution can be valid in some cases, such as pure projection geometry, focusing by a thin lens, diffraction at one slit, etc.

\[ I_\omega (x, y) \approx \int \tilde{I}_{\omega1} (x - \tilde{x}_e, y - \tilde{y}_e) \tilde{f}(\tilde{x}_e, \tilde{y}_e) \, d\tilde{x}_e \, d\tilde{y}_e \]

If convolution is valid, the calculations can be accelerated dramatically. The validity of the convolution relation can be easily verified numerically.
Updates of Core SRW Functions
Made at NSLS-II (in collaboration with other Labs)

- Accurate partially-coherent emission and wavefront propagation simulations for SR sources are possible with SRW since ~2009:

- Parallel calculations of Partially-Coherent Emission and Wavefront Propagation are implemented in SRW for Python (based on MPI / mpi4py). Besides “normal” Intensity, calculation of Mutual Intensity / Degree of Coherence is possible:

- Increased reliability of Time- / Frequency-Dependent FEL Pulse Propagation simulations:

- New physical-optics “propagators” are implemented for:
  - Grazing-Incidence Focusing Mirrors, using the stationary phase method / “local ray-tracing”:
  - Perfect Crystals, using the X-ray Dynamical Diffraction methods:
  - Variable Line Spacing Gratings, using the stationary phase method:
R&D Direction: Improvement of efficiency and reliability of Partially-Coherent “Forward” Simulation

NSLS-II Hard X-Ray Nanoprobe (HXN) Beamline Optical Scheme and Wavefront Propagation Simulation

Flux after HCM: \(\sim 7.4 \times 10^{14}\) ph/s/.1%bw

Flux within N.O. Aperture (d=150 μm): \(\sim 3.6 \times 10^{12}\) ph/s/.1%bw

IVU20  HCM  MONO  HFM  SSA

N.O.: ZP or MLL

Sample Plane

Horizontal Plane

Vertical Plane

Y. Chu, H. Yan, K. Kaznatcheev

Pan-Am SRI-2010

Intensity Distributions
Final Focal Spot Size and Flux at Sample vs Secondary Source Aperture Size (HXN, NSLS-II)

Horizontal Spot Size and Flux vs Horizontal Secondary Source Aperture Size

Vertical Spot Size and Flux vs Vertical Secondary Source Aperture Size

$\Delta y_{ss} = 30\, \mu m$

$\Delta x_{ss} = 20\, \mu m$

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, $D = 150\, \mu m$ located at 15 m from Secondary Source (109 m from Undulator)
Intensity Distributions at Sample for Different Secondary Source Aperture Sizes at HXN (NSLS-II)

In Horizontal Median Plane ($y = 0$)

For Different Horizontal SSA Sizes ($\Delta x_{ss}$)

For Different Vertical SSA Sizes ($\Delta y_{ss}$)

In Vertical Median Plane ($x = 0$)

For Nanofocusing Optics with $F = 18.14$ mm, $D = 150$ μm ($\Delta r \approx 15$ nm; $E_{ph} \approx 10$ keV)

SSA located at 94 m, Nanofocusing Optics at 109 m from Undulator
Partially-Coherent Wavefront Propagation Simulations for a Beamline with Grazing-Incidence Focusing Mirrors, Taking Into Account Their Imperfections (FMX @ NSLS-II)

**Horizontal SSA Size:** 30 μm  
**Photon Energy:** 12.7 keV  
**Flux at Sample:** \(~5.4 \times 10^{13} \text{ ph/s/1%bw}\)

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**Mirror Slope Error**

**Mirror Height Profile Error**

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**KB simulated using Grazing-Incidence “Thick Optical Element” Propagator based on “Local Ray-Tracing”.**  
**KB Surface Height Error simulated by corresponding Phase Shifts (“Masks”) in Transverse Plane at Mirror Locations.**

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**Intensity Distributions at Sample**

**Without Mirror Errors**

**With Mirror Errors**

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**hor. cuts \((y = 0)\)**

**vert. cuts \((x = 0)\)**
Using CRL for Producing “Large Spot” at Sample of FMX Beamline @ NSLS-II

**Source:**
- Electron Current: 0.5 A
- Horizontal Emittance: 0.55 nm (“ultimate”)
- Vertical Emittance: 8 pm
- Undulator: IVU21-1.5 m centered at +1.25 m from Low-Beta Straight Section Center

**CRL “Transfocator”:**
- **8 Horizontally** + **3 Vertically-Focusing Be Lenses**
- \( R_{\text{min}} = 200 \, \mu m \)
- \( F_h \approx 5.9 \, m, \; F_v \approx 15.8 \, m \)
- Geom. Ap.: 1 mm x 1 mm
- Located at 0.75 m before VKB edge
  (10 m after SSA)
- Flux Losses at CRL: ~1.6 times

Horizontal SSA Size: 30 μm
Photon Energy: 12.7 keV

Intensity Distributions at Sample

Without Mirror Errors

With Mirror Errors

**Electron Beam Distribution:**
- Photon Energy: 12.7 keV
- Horizontally (y = 0)
- Vertically (x = 0)
Partially-Coherent Wavefront Propagation Simulations for CHX Beamline @ NSLS-II

Intensity Distributions for $E = 10$ keV
$\Delta S_{1x} = 44 \mu m$
$\Delta S_{1y} = 1 mm$

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
Introducing Intensity Distribution and Degree of Transverse Coherence at a Sample (CHX @ NSLS-II)

**Intensity Distribution**

- **In Horizontal Mid-Plane**
  - Vertical Position vs. Horizontal Position
- **In Vertical Mid-Plane**
  - Similarly structured, but with an orientation change.

**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**
- **In Vertical Plane**

Mathematical Expressions:

\[ \mu(r_1, r_2, \omega) = \left| \frac{W(r_1, r_2, \omega)}{[W(r_1, r_1, \omega)W(r_2, r_2, \omega)]^{1/2}} \right| \]

\[ W(r_1, r_2, \omega) \sim \langle E(r_1, \omega)E^*(r_2, \omega) \rangle \]

Graphical Representations:

- Graphs illustrating intensity and coherence length comparisons:
  - Horizontal Coherence Length: \(~9.4\ \mu m\)
  - Vertical Coherence Length: \(~13.4\ \mu m\)

**Observation**

- Good agreement with 2-slit interference simulation results.

**Conclusion**

The study confirms the theoretical predictions with experimental data collected at the sample (CHX @ NSLS-II), providing a comprehensive analysis of intensity and coherence characteristics.
Partially-Coherent Wavefront Propagation Simulations for Inelastic X-ray Scattering Beamline with Advanced High-Resolution Crystal Optics (IXS @ NSLS-II)


Extended testing of new Physical Optics Propagator for Crystals

IXS Monochromators contain:
- DCM: 2 Crystals
- HRM: 4 Crystals of HRM

Mirror Surface Error is not taken into account

\[ E_0 \approx 9131.7 \text{ eV} \]
Partially-Coherent Wavefront Propagation Simulations for a Soft X-ray Beamline with VLS grating (ESM @ NSLS-II)

Beamline Design:

Part.-Coherent Wavefront Propagation Simulations:

In these simulations, the horizontal secondary source slit size was set to be equal to the vertical size ($\Delta x = \Delta y$); mirrors' height / slope errors were not taken into account (to be included in next series of simulations).

Energy Resolution as functions of the Secondary Source (Monochromator Exit) Slits

Spatial Resolution

Flux (finite-bandwidth) at Sample

Two different VLS Gratings (160 mm long) were used:
$\alpha_0 = 800$ lines/mm for $E = 20$ eV; $\alpha_0 = 600$ lines/mm for $E = 60, 100$ eV
Approach to Coherence Preservation Diagnostics Assisted by Simulations (Illustration)


Optical scheme of test experiments with CRL and a Boron fiber probe

**U33 (APS 32ID)**

**Mono**
- $E_{ph} = 8.5$ keV

**1D Be CRL**
- 1 – 5 lenses
- $R_{\text{min}} = 500$ μm
- $D = 1$ mm

**B-Fiber**
- $D = 100$ μm

**Detector**
- YAG + CCD

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- ~1.25 m from center of straight section
- ~36 m
- ~71 m
- ~75 m
Intensity Distributions in the B-fiber Based Interference Scheme for Different Numbers of CRL in Optical Path

Simulations allow to conclude about coherence preservation in presence of any beamline optics!

### Measurement
- **1 lens**
- **2 lenses**
- **3 lenses**
- **5 lenses**

### Calculation
- **1 lens**
- **2 lenses**
- **3 lenses**
- **5 lenses**

**vertical cuts (at x = 0)**
Intensity Distributions of Focused Wiggler Radiation from Partially-Coherent Wavefront Propagation Calculations

On-Axis Collection: $\theta_x = 0$, $\theta_y = 0$
$|\theta_x - \theta_x^0| < 0.1 \text{ mrad}$
$|\theta_y - \theta_y^0| < 0.1 \text{ mrad}$

Off-Axis Collection: $\theta_x = 0.5 \text{ mrad}$, $\theta_y = 0$

$\theta_x = 1 \text{ mrad}$, $\theta_y = 0$

1:1 Imaging Scheme with “Ideal Lens”

NSLS-II Low-Beta Straight Section
$I = 0.5 \text{ A}, \varepsilon_x = 0.9 \text{ nm}, \varepsilon_y = 8 \text{ pm}$

SCW40: $\lambda_u = 40 \text{ mm}, B_{\text{max}} = 3 \text{ T}, L = 1 \text{ m}$
Photon Energy: $E_{\text{ph}} = 10 \text{ keV}$
Intensity Distributions of Monochromatic Radiation from ESRF-U 2PW in 1:1 Imaging Plane

“Non-saturated” Image Plot:
From Downstream Dipole (out of focus)
(max. intensity 50 times lower than in the “non-saturated” plot)

“Saturated” Image Plot:
From 2PW (well focused)

Focusing by Ideal Lens located at: R = 30 m
Lens Aperture: Δx = 8 mm, Δy = 10 mm
Photon Energy: 5 keV

Cuts by Horizontal Median Plane
Cuts by Vertical Plane (x = 0)

at Different Horizontal Apertures
Estimating Degree of Coherence (/ Transverse Coherence Lengths) of Radiation from ESRF-U 2PW by Simulating Young’s 2-Slit Interference Schemes

Far-Field Interference Patterns from 2 Vertical Slits Separated by Horizontal Distance h

Fringe Visibility vs h in Horizontal Plane

Vertical Aperture: 1 mm; Slit Size: 2 µm
Horizontal Coherence Length: ~40 µm
For a BM-like Source should be ~60 µm

Far-Field Interference Patterns from 2 Horizontal Slits Separated by Vertical Distance h

Fringe Visibility vs h in Vertical Plane

Horizontal Aperture: 1 mm; Slit Size: 2 µm
Vertical Coherence Length: ~390 µm
For a BM-like Source should be ~390 µm

\[ \text{Fringe Visibility} = \frac{1}{1 + \frac{\sigma_v^2}{2}} \]

\[ E_{ph} = 5 \text{ keV} \]
\[ R = 30 \text{ m} \]
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