# Computer simulations for X-ray optics with XOPPY

***TUTORIALS on XOPPY (EXERCISES AND ANSWERS)***

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Spectral characteristics of synchrotron sources and characteristics of optical elements (Exercises to be done with XOPPY)

* Emission characteristics of synchrotron radiations sources
  1. Bending magnets
  2. Conventional wigglers
  3. Non-conventional wiggler (asymmetric and short)
  4. Undulator sources (angular distribution)
  5. Undulator sources (flux and spectral density)
* 6.- Filters and mirrors: effect on source: absorbed and transmitted power by mirrors and attenuators
* 7.- Crystal monochromators: diffraction profiles of a single and multiple reflections. Rocking curves. Harmonic rejection.
* 8.- Bent crystals: diffraction profiles. Transition from dynamical to kinematical theory
* 9.- Compute reflectivity curves of multilayers
* 10.- Quick tour to other applications

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### emission characteristics of synchrotron radiations sources: Bending Magnets

You will learn:

* to calculate bending magnet spectra using BM

Simulate bending magnet spectra for different BM sources at ESRF. Calculate numerical values for the different values of magnetic field. Fill them in the table below. Considering 1 mrad of horizontal aperture.

1. Values of critical energy
2. Flux in number of photons at critical Energy
3. Total power emitted by the BM in the full energy range.

Try to remember and check (or guess from numerical values)

iv) How the total power scales with the electrons energy?

v) What is the power in the energy range from zero to the Ec? and from Ec to infinity?

Hints:

* Use *XOPPY|BM*
* The questions iv) and v) can be answered without using the computer.

***Answer***

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Facility** | **E [GeV]** | **I [mA]** | **B [T]** | Ec [eV] | i (Flux) | ii (Total Power [W]) |
| **ESRF** | **6** | **200** | **0.856** | 20492 | 12.7+132.72e13 | 153.87149.9 |
| **EBS-DQ1D** | **6** | **200** | **0.55** | 1316719414 | 12.7+132.72e13 | 100.33149.9 |
| **EBS-DQ2C** | **6** | **200** | **0.4** | 951619414 | 12.7+132.72e13 | 73.06149.9 |

iv) How the total power scales with the electrons energy?

Proportional to E4 when keeping constant the bending radius R

v) What is the power in the energy range from zero to the Ec? and from Ec to infinity? P[0,Ec]=P[Ec,∞]=0.5 Total Power

##### Angular distribution. Polarization

### emission characteristics of synchrotron radiations sources: Conventional wigglers and short wigglers

You will learn:

* to calculate standard wiggler spectra using WIGGLER and WS.
* understand the differences between these programs
* to calculate the flux of short wiggler spectra using WIGGLER
* Use magnetic field from B(y) map or from harmonic decomposition.

Simulate spectra for different ESRF *conventional* wigglers. Calculate

1. Maximum flux (for I=200 mA)
2. Critical Energy corresponding to maximum deflection
3. Calculate the effective critical energy
4. Total emitted power (for I=200 mA)

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **u[m]** | **K** | **N** | Max Flux  ph/sec/0.1%bw | Ec [eV] | Tot Power at I=200 mA  [kW] |
| **Id17** | **0.150** | **21.015** | **10** | 3.03e19 | 20204  web:20000 | 4.86  web 4.74 |
| **SW3P** |  |  |  | 1.58e15 at 5.1keV  (1.4e17??) | 30631  (web 29000) | 10.415  (web:20) |

Used symbols:

u: magnetic period of the insertion device

N: number of periods

K: deflection parameter

Information source:

ID17 W150 parameters at SYNED file: <http://ftp.esrf.fr/pub/scisoft/syned/lightsources/ESRF_ID17_EBS_HPW150_2.json>

Magnetic field for SW3P can be found at:

<http://ftp.esrf.fr/pub/scisoft/syned/resources/SW_3P.txt>

***Answer***

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **u[m]** | **K** | **N** | **Bmax**  **[T]** | Max Flux  ph/sec/0.1%bw | Ec [eV] | Tot Power at I=200 mA [kW] |
| **Id9** | **0.070** | **5.43** | **22** | **0.83** | 1.06e15 | 20204  web:20000 | 4.86  web 4.74 |
| **Id11** | **0.125** | **14.7** | **12** | **1.24** | 1.58e15 at 5.1keV  (web 1.4e17??) | 30631  (web 29000) | 10.415  (web:20) |
| **Id17** | **0.150** | **19.6** | **11** | **1.5-1.4** | 2.11e15 | 34034  (web:33500) | 13.9  (web:14.3) |

Note that

1) WIGGLER generates the full emission of the wiggler versus photon energy (i.e., integrated over the full emission angle)

2) WS creates emission either integrated over a given aperture area placed at a given distance, or integrated over given emission angle (set the distance to zero in this case). Note that for comparison with WIGGLER the slit must be large enough to receive the full emission. However, very large aperture will result in inaccurate calculations because the integral is doing over a mesh with few points in X and Y (max 50×50).

Advanced notes:

* It is not possible to calculate flux on a slit for a given magnetic field (WS does not accept external field). Make ray tracing Wiggler simulation, use a slit to compute the acceptance, and rescale the spectrum. See e.g., <https://gitlab.esrf.fr/srio/ebs-readiness/blob/master/bm05/scan_energies.py>
* External magnetic field can be given as an harmonic decomposition (Exercise: calculate the harmonic decomposition of SW3P)
* Power Density for wigglers can be calculated using the UndulatorPowerDensity wiggler
* If you want to calculate electron trajectory and velocity, the ShadowOui/Wiggler widget can be used

Calculate the harmonics starting from B(T)

### emission characteristics of synchrotron radiations sources: Undulator sources (flux and spectral power, tuning curves)

You will learn:

* to calculate the photon flux, spectral power and total power emission of undulators
* to calculate and visualize the effect of electron beam emittances (EBS vs ESRF)

i) Calculate the flux and spectral power spectra for an U18 undulator placed at the EBS straight section (e.g., ID06) and at the old ESRF high beta section (ID06) and old ESRF low beta section (ID11). Use a 3×3mm2 slit placed at 30 m from the source. Give the maximum flux and total power. Reduce the slit dimension.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | N | K | *u* [mm] | Power [W] | Flux |
| U18 EBS | 111 | 1.5 | 3x3 |  |  |
| U18 High Beta | 111 | 1.5 | 3x3 |  |  |
| U18 Low Beta | 111 | 1.5 | 3x3 |  |  |

Hints: Use Undulator Spectrum. Compare results of the different codes.

|  |  |  |  |
| --- | --- | --- | --- |
|  | High Beta | Low beta | EBS |
| *x* [m] | 414.97 | 50.40 | 30.18 |
| *z* [m] | 3.43 | 3.44 | 3.64 |
| *x’*[rad] | 10.31 | 107.19 | 4.37 |
| *z’*[rad] | 1.16 | 1.16 | 1.37 |

Source: <http://ftp.esrf.fr/pub/scisoft/syned/README.txt>

***Answer***

i) Use the files:

ii) For comparison,

Advanced notes:

* K= B B=f(gap) with f depending on the device
* L0 = … E0 =
* Change K -> Change Peak -> Tunning curves

### emission characteristics of synchrotron radiations sources: Undulator sources (power density)

You will learn:

* to calculate the spatial distribution of power emitted by an undulator or wiggler using Undulator Power Density
* Project it on a (plane) optical element
* Approximate the distribution with a Gaussian function.

Calculate the flux and spectral power spectra for an U18 undulator placed at the EBS straight section (e.g., ID06) at 30 m from the source

Hint: Use a slit large enough to include all the power.

***Answer***

### emission characteristics of synchrotron radiations sources: Undulator emission vs (x,y,E)

You will learn:

* to calculate the monochromatic angular distribution of the undulator emission using Undulator Radiation

a) Calculate the distribution of flux (at an energy corresponding to the first harmonic, E=166.8 eV) versus emission angle for the yellow book example (no emittance, N=14, *Ee*=1.3 GeV, *u*=3.5cm, K=1.87). Use Xurgent and Xus

b) Calculate the flux and spectral power spectra for an U18 undulator placed at the EBS straight section (e.g., ID06) at 30 m from the source

***Answer***

Use the XOP input files:

Advanced notes:

* Resonance and flux peak separate when slit opens: Eo is a function of angle
* At resonance the emission is smooth (Gaussian-like?) Approximated divergence sigma = sqrt(lambda/(2L))
* At the peak a dip??? May appear

--surface plot of power

--K(gap) (check with id21 application)

--TC see http://www.esrf.fr/machine/support/ids/Public/Brilliance/brilliance.html

--Angular distribution Power map on a screen and on a mirror (after upgrading xsurface1)

### Attenuators and mirrors: effect on source

You will learn:

* to calculate attenuator transmission and mirror reflectivity and to see their effects on the source spectrum.
* evaluate absorbed and transmitted power
* calculate the effect of attenuators and mirrors in power density

Calculate how a 500 m Be window plus a Rh mirror (set at 3 mrad of grazing angle) modify the BM flux calculated in the previous exercise 1. Calculate the absorbed power by these elements. Add other filters (e.g., Al, Mo, etc).

Hints: From the *Xop|BM* window used previously, create the files with the source spectra by using *BM|File|Write files for xop/Optics*. Open the *Xop|Optics|Mirrors&Filteres|XPOWER* application. From the main parameter window, select the source to either *xop/source Flux* or *xop|source Power*. Fill-in the optical elements parameters. The items in the *XPOWER|Show* menu will present the results. Use *Show|Cumulative transmission* to see the sequential effect of the optical elements on the source. Use the *Xplot|Save* button to over plot the spectra after the different elements.

***Answer***

use the XOP input file ex6\_xpower.xop Dashed line: source. Dotted line: after Be filter. Continuous line: after Be filter and Rh mirror. See absorbed and transmitted power using Show|Parameters

D:\Working\SPIECourse\FIGS\ex6p.eps

### Crystal monochromators

You will learn:

* calculate diffraction profiles of perfect crystals
* calculate the response of two crystals (+,-) (curve multiplication)
* calculate rocking curves (convolution)
* calculate harmonic suppression

i) Calculate the diffraction profiles, Bragg angle, width, peak and integrated reflectivity of Si 111 at the energies 5 keV, 8 keV, 12 keV, 50 keV, 80 keV and 120 keV.

ii) For the 8 keV case, calculate the diffracted profile of a double Si111 reflection in (+,-) configuration. Calculate the rocking curve resulting of the rotation of the second crystal respect to the first one.

iii) For a Si111 double crystal monochromator at 8 keV, calculate the angular tilt of the second crystal needed to suppress the third harmonic reflection.

Hints: Use the *Xop|Optics|Crystals|XCrystal* application to create the profiles. The peak, width and integrated reflectivity values can be obtained using *Xplot|Calculations|Width/Integral/MinMax* on each profile. For the double reflection (+,-) one should multiply a given diffraction profile by itself using the *Xplot|Calculations|Operations with columns* item. Use *Xplot|Save Plot* button to over plot the new curve on the original one. The rocking curve is calculated by convoluting the diffraction profile with itself. For doing that, use the *Xplot|Calculations|Convolution and Correlation* entry, and make autoconvolution normalized to the second set.

For the harmonic suppression one should calculate the main Si111 reflection at 8 keV and the third harmonic (Si333 at 24 keV). Check that both cases give the same Bragg angle. Keep two Xplot windows, one for each profile. Estimate the misalignments one must introduce to suppress the Si333 reflection (should be larger than the diffraction profile width). Create a new set of data for the shifted Si333 reflection by changing the angular (abscissas value with *Xplot|Calculations|Operations with sets*. Save the result to a file. Multiply the original Si333 reflection by the shifted one using the *Xplot|Calculations|Operations with sets* of the Xplot window of the original Si333 Xplot window. Repeat the process of shifting with the main reflection Si111 using the same value of angular misalignment. Calculate the new peak, width and integrated reflectivity, and compare with the double non-misaligned reflection (+,-).

***Answer***

i)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Crystal | E [keV] | B [deg] | W[rad] | Peak | Integ Int |
| Si111 | 5 | 23.3 | 61.3 | 0.86, | 60 |
| Si111 | 8 | 14.3 | 36.5 | 0.94, | 40 |
| Si111 | 12 | 9.5 | 23.8 | 0.97, | 28 |
| Si111 | 50 | 2.27 | 5.55 | 1.00, | 6.7 |
| Si111 | 80 | 1.42 | 3.48 | 1.00, | 4.2 |
| Si111 | 120 | 0.94 | 2.31 | 1.00, | 2.9 |

ii) Continuous line: convolution (rocking curve). Dashed line: single reflection. Dotted line: double reflection

..\..\..\..\Program Files\XOP2.0\tmp\rockcurvep.eps

iii)

Si333 single reflection: W=3.1, P=0.99, I=3.45 => Shifting 3.5 rad

Si333.Si333(shifted): W=3.1, P=0.07, I=0.24

Si111.Si111: W=33.8, P=0.88, I=29.2

Si111.Si111(shifted): W=32.3, P=0.88, I=28.4

### Bent crystals

You will learn:

* to calculate diffractions profiles of bent crystals
* understand the limitations of the available models
* to see the transition from dynamical to kinematical theory

i) Calculate the deformation of Si111 symmetric Bragg diffraction profile at 12 keV for different values of the bending radius (from 100m to 5cm). For each curve calculate the integrated reflectivity and see the transition from the Dynamic theory value (R>>) to the Kinematical theory value (R<<).

ii) Calculate the diffraction profile in Laue for Si111 at 33 keV and asymmetry angle a=63.78 deg, and curvature radius 13m.

Hints: Use *Xop|Crystals|Crystal\_bent* application. Use the “multilamellar” theory for the Bragg reflection and the “Penning&Polder” theory for the Laue system.

Use the files ex8\_xcrystal\_bent.xop and ex8\_xcrystal\_bent\_bragg.xop for examples for Laue and Bragg configurations, respectively.

***Answer***

i)

|  |  |  |
| --- | --- | --- |
| R[cm] | FWHM[mrad] | Integrated reflectivity |
| 5 (dashed) | 92 | 0.395 |
| 25 | 0.39 | 0.300 |
| 50 (dotted) | 0.19 | 0.22 |
| 100 | 0.11 | 0.136 |
| 2000 (cont) | 0.03 | 0.97 |

..\..\..\..\Program Files\XOP2.0\tmp\xcrystal_bent_braggp.eps

ii)

..\..\..\..\Program Files\XOP2.0\tmp\xcrystal_bent_lauep.eps

### Reflectivity curves of multilayers.

You will learn to:

* use Mlayer to calculate reflectivity from simple multilayers
* understand the limitations of Mlayer
* start and use IMD as Xop extension
* understand the basic features of multilayer reflectivity spectra

i) Using MLAYER calculate the reflectivity as a function of grazing angle, from zero to 6 deg, of [W (25 Å)/Si (25 Å)]×50 on Si at an energy of 8050 eV

ii) Using IMD, using no slope errors (if not specified), calculate the following reflectivity spectra at E=8050 eV:

1. [W (25 Å)/Si (25 Å)]×50 on Si
2. [W (10 Å)/Si (40 Å)]×50 on Si
3. [W (5 Å)/Si (45 Å)]×50 on Si
4. [W (25 Å)/Si (25 Å)]×10 on Si
5. [W (25Å)/Si (25 Å)]×50 on Si, roughness =5 Å
6. SiO(90 Å) [W (5 Å)/Si (45 Å)]×50 on Si

Comment the results.

Hints: load in IMD the input file ex9\_imdWSi.dat which contains an input for the Wsi multilayer

***Answer***

i) Use the file ex9\_mlayer.xop

ii) Start with the file ex9\_imdWSi.dat.

The following features can be observed:

1) A plateau corresponding to the total reflection zone.

2) Outside the plateau, the background decreases with q-4. Changes in this background are due to the roughness in the interfaces and experimental background.

3) Satellite maxima. The angular spacing depends on the bilayer periodicity d. Their angular separation is determined by the Bragg law. If the spectrum extends over many peaks, it is possible to observe absences of some peaks, which are related to Γ. Peaks at Γ-1 are absent.

4) Kiessig fringes, which period depends on the total multilayer thickness (i.e., number of bilayers).

5) If a top or capping layer exists (usually an oxide layer) it creates side maxima close to the satellites.

6) The satellite width is proportional to 1/N, N being limited by the absorption of the stack. Although the theoretical width is the same for all satellites, in experimental measurements one usually sees an increase of the satellite width as the satellite order increases.

7) The effect of increasing N is also to increase peak intensity in satellites. This is limited by the roughness and stack absorption.

..\..\..\..\Program Files\XOP2.0\tmp\imd1p.eps..\..\..\..\Program Files\XOP2.0\tmp\imd2p.eps

3

2

1

..\..\..\..\Program Files\XOP2.0\tmp\imd3p.eps..\..\..\..\Program Files\XOP2.0\tmp\imd4p.eps

4

3

3

3

..\..\..\..\Program Files\XOP2.0\tmp\imd5p.eps..\..\..\..\Program Files\XOP2.0\tmp\imd6p.eps

5

4

3

2

1

### Quick tour to other XOPPY applications

Open and run the following applications:

* XRAYLIB
* XCOM
* MARE