

XOP tutorial at ESRF - Session 1

Introduction to XOP

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emission characteristics of synchrotron radiations sources

1. Bending Magnets

You will learn:

- to calculate bending magnet spectra using BM
- the basic use of Xplot

Simulate bending magnet spectra for different sources. Calculate numerical values, and fill them in the table below.

i) Maximum flux in number of photons (considering 1 mrad of horizontal aperture)

ii) Total power emitted by the BM in the full energy range.

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

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

iv) What is the power in the energy range from zero to the E_c ? and from E_c to infinity?

Facility	E [GeV]	I [mA]	B [T]/R[m]	E_c [eV]	i (Flux)	ii (Total Power [W])
ESRF	6.04	200	0.8/ 25.2			
Elettra	2	300	1.2/ 5.56			
LNLS	1.37	175	1.67/ 2.74			
SLS	2.4	400	1.45 & 5/ 5.52 & 1.6			
APS	7	100	0.6/ 38.9			
NSLS	2.58	500	0.77/ 11.2			
SSRL	3	100	1.22/ 8.20			

Information source:

ESRF: www.esrf.fr

Elettra: <http://www.elettra.trieste.it/about/parameters.html>

LNLS: <http://www.lnls.br/info/info.htm>

SLS: http://www1.psi.ch/www_sls_hn/sls_accelerator.htmlx

Others: <http://www-als.lbl.gov/als/intersrc/existing.html>

Hints:

Use *XOP/Bending Magnet /BM* to create the spectra. Numerical values can be obtained from the resulting *BM/Show/View Results* window and plots can be done using *BM/Show/Plot Results*, which creates a graphical window (Xplot). Power values can be calculated by integrating the power density spectra or read directly from the results window.

Integration of the power spectrum can be done with *Xplot/Calculations/Width/Integral/MinMax* menu. For integrating over a limited range of abscissas, just select the desired interval with *Xplot/Edit/Limits/Set...* and then apply the *Xplot/Calculations/Width/Integral/MinMax* again.

The questions iii) and iv) can be answered without using the computer. Question iv) can be checked by calculating the normalized cdf(power spectrum) using first *Xplot/Calculations/cdf* to calculate cdf(power spectrum) and then normalizing the result with *Xplot/Calculations/Operations with columns*

2. Conventional wigglers

You will learn:

- to calculate standard wiggler spectra using Xwiggler and WS.
- understand the pros and cons of each program
- use applications input files

Simulate spectra for different ESRF *conventional* wigglers. Calculate

- Maximum flux (for I=200 mA)
- Critical Energy corresponding to maximum deflection (from *Show parameters*)
- Calculate the effective critical energy with Xplot
- Total emitted power (for I=200 mA)

	λ_u [m]	K	N	Max Flux ph/sec/0.1%bw	Ec [eV]	Tot Power at I=200 mA [kW]
Id9	0.070	5.43	22			
Id11	0.125	14.7	12			
Id17	0.150	19.6	11			

Used symbols:

λ_u : magnetic period of the insertion device

N: number of periods

K: deflection parameter

Information source: http://www.esrf.fr/machine/support/ids/Public/Ids/installed_IDS.html
and beamline web pages

Hints: Use the Xop|Sources|wigglers|Xwiggler to create the spectra. Make calculations, for instance, from 100 to 100000 eV with 200 eV step. Save the flux spectrum of id9 in an ASCII file (for comparison with results of undulator model, to be done later).

Use the Xop|Sources|wigglers|Ws for calculating the spectrum of id11. Compare with previous results.

Use Xplot|Calculations|Width/Integral/MinMax to get maxima. The effective critical energy can be calculated using the normalized cdf(flux), as done before.

3. Asymmetric wiggler (id20)

You will learn:

- to calculate the flux of asymmetric wiggler spectra using Xwiggler
- Use magnetic field from B(y) map or from harmonic decomposition.

Calculate the emission spectrum of an asymmetric wiggler

- Calculate the maximum flux and the total emitted power XWIGGLER
- Calculate B as a function of the harmonics (use Xop|Tools|Xop macro, load and run the file xwiggler_id20.mac)

	λ_u [m]	K	N	Max ph/sec/0.1%bw	Flux*	Ec [eV]	Tot Power* [kW]
Id20(asym)	0.210	15	8				

Hints: Use Xop|Xwiggler. The magnetic field data for Id20 is available in the files xwiggler_h.dat or xwiggler_b.dat (harmonics and magnetic field, respectively).

4. Undulator sources (angular distribution)

You will learn:

- to calculate the angular distribution of the undulator emission using Xurgent and Xus
- to calculate and visualize the effect of electron beam emittances.

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, $N=14$, $E_e=1.3$ GeV, $\lambda_u=3.5$ cm, $K=1.87$). Use Xurgent and Xus

ii) Calculate the distribution of flux (at an energy corresponding to the first harmonic) versus emission angle for ESRF U46 ($E_e=6.04$ GeV, $N=35$, $\lambda_u=46$ mm, $K=2.76$) in three cases: i) no emittance, ii) undulator placed in an ESRF high beta section, and iii) low beta. Use Xus (and Xurgent)

	High Beta	Low beta	BM
σ_x [μm]	395	57	126
σ_z [μm]	9.9	10.3	36.9
σ_x' [μrad]	10.5	88.3	108
σ_z' [μrad]	3.9	3.8	1.1

Information source: <http://www.esrf.fr/machine/support/ids/Public/Sizes/sizes.html>

5. Undulator sources (flux and spectral density)

You will learn:

- to calculate the photon flux, spectral density and total power emission of undulators

i) Calculate the flux and spectral power spectra for the three insertion devices of id9 (low beta). Use a $3 \times 3 \text{ mm}^2$ slit placed at 27 m from the source. Give the maximum flux and total power.

ii) Compare the W70 flux with the result obtained with the wiggler model.

	N	K	[mm]	Power [W]	Flux
U20	81	0.27	20	45.5	6.38e13
U46	36	2.76	46	571.8	1.88e14
W70	22	5.43	70	472.0	9.45e13

Hints: Use Xop|Sources|Undulator|Xurgent and/or Xop|Sources|Undulator|Xus. Compare results. Check power results with web data at: http://www.esrf.fr/exp_facilities/ID9/id9.html

6. Filters and mirrors: effect on source

You will learn:

- to save an Xop source to files to be used with Xpower
- to calculate filter transmission and mirror reflectivity and to see their effects on the source spectrum.
- evaluate absorbed and transmitted power

Calculate how a 500 μm 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 overplot the spectra after the different elements.

7. 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 overplot 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 (+,-).

8. 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 ($R \gg$) to the Kinematical theory value ($R \ll$).

ii) Calculate the diffraction profile in Laue for Si111 at 33 keV and asymmetry angle $\alpha=63.78$ 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.

9. 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 $[W (25 \text{ \AA})/Si (25 \text{ \AA})] \times 50$ 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. $[W (25 \text{ \AA})/Si (25 \text{ \AA})] \times 50$ on Si
2. $[W (10 \text{ \AA})/Si (40 \text{ \AA})] \times 50$ on Si
3. $[W (5 \text{ \AA})/Si (45 \text{ \AA})] \times 50$ on Si
4. $[W (25 \text{ \AA})/Si (25 \text{ \AA})] \times 10$ on Si
5. $[W (25 \text{ \AA})/Si (25 \text{ \AA})] \times 50$ on Si, roughness $\sigma=5 \text{ \AA}$
6. SiO(90 \text{ \AA}) $[W (5 \text{ \AA})/Si (45 \text{ \AA})] \times 50$ on Si

Comment the results.

10. Quick tour to other applications

Open and run the following applications:

- DABAX main interface and applications
- XXCOM
- MAMON
- CRL

Appendix – Useful formulas

Bending Magnet:

$$E[eV] = \frac{12398.52}{\lambda[\text{\AA}]} \quad (1.1)$$

$$\gamma = \frac{E_e}{m_e c^2} = \frac{E_e[\text{GeV}]}{511.0034 \cdot 10^{-6} \text{GeV}} = 1956.93 E_e[\text{GeV}] \quad (1.2)$$

$$B[T] = \frac{3.334728 E_e[\text{GeV}]}{R[m]} \quad (1.3)$$

Critical energy and wavelength

$$\lambda_c = \frac{4\pi R}{3 \gamma^3}; \quad E_c[\text{keV}] = 0.665 E_e^2[\text{GeV}] B[T] \quad (1.4)$$

Power emitted

$$P[\text{W} / \text{mrad}] = \frac{88.46278 E_e^4[\text{GeV}] I[\text{A}]}{2\pi R[m]} \quad (1.5)$$

Wiggler and Undulators:

$$K = 0.934 \lambda_u[\text{cm}] B[T] \quad (1.6)$$

First harmonic energy:

$$\varepsilon_1[\text{keV}] = 0.950 \frac{E^2[\text{GeV}]}{\left(1 + \frac{K^2}{2}\right) \lambda_u[\text{cm}]} \quad (1.7)$$

Central cone width of the n -th harmonic:

$$\sigma_{r'} = \frac{1}{\gamma} \sqrt{\frac{1 + \frac{K^2}{2}}{2Nn}} = \sqrt{\frac{\lambda/n}{L}} \quad (1.8)$$

Position of the l -th ring:

$$\theta_{n,l} = \frac{1}{\gamma} \sqrt{\frac{l}{n} \left(1 + \frac{K^2}{2}\right)} \quad (1.9)$$

Total radiated power

$$P[\text{kW}] = 0.633 E^2[\text{GeV}] B_0^2[T] L[m] I[\text{A}] \quad (1.10)$$

Answers

1 – Bending magnets

Use the XOP input files `bm_*.xop`

Facility	E [GeV]	I [mA]	B [T]/R[m]	E_c [eV]	i (Flux)	ii (Total Power [W])
ESRF	6.04	200	0.8/ 25.2	19414	2.72e13	149.9
Elettra	2	300	1.2/ 5.56	3193	1.34e13	12.16
LNLS	1.37	175	1.67/ 2.74	2085	5.41e12	3.17
SLS	2.4	400	1.45 & 5/ 5.52 & 1.6	5555.7& 19158	5.41e12& 2.16e13	33.87& 116.8
APS	7	100	0.6/ 38.9	19557	1.58e13	86.9
NSLS	2.58	500	0.77/ 11.2	3409.4	2.90e13	27.9
SSRL	3	100	1.22/ 8.20	7303.8	6.77e12	13.91

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

Proportional to E^4 when keeping constant the bending radius R

iv) What is the power in the energy range from zero to the E_c ? and from E_c to infinity? $P[0,E_c]=P[E_c,\infty]=0.5$ Total Power

2 – Conventional wigglers

use the XOP input files:

`xwiggler_id9.xop`
`xwiggler_id11.xop` and `ws_id11.xop`
`xwiggler_id17.xop`

	λ_u [m]	K	N	Bmax [T]	Max Flux ph/sec/0.1%bw	E_c [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)

3 – Asymmetric wiggler (id20)

Use the XOP input files:

`xwiggler_id20_b.xop`
`xwiggler_id20_h.xop`

	λ_u [m]	K	N	Bmax[T]	Max ph/sec/0.1%bw	Flux*	E_c [eV]	Tot Power* [kW]
Id20(asym)	0.210	15	8	0.9	1.58e15		(19000) 11200 22465	(2.2) 1.597

4 – Undulator sources (angular distribution)

Use the XOP input files:

xurgent_yellowbook.xop and xus_yellowbook.xop

xurgent_hb_u46.xop and xus_hb_u46.xop

xurgent_lb_u46.xop and xus_lb_u46.xop

In Xus the results are under Xus|Show|Plot 3D surface|Total intensity

5 – Undulator sources (flux and spectral density)

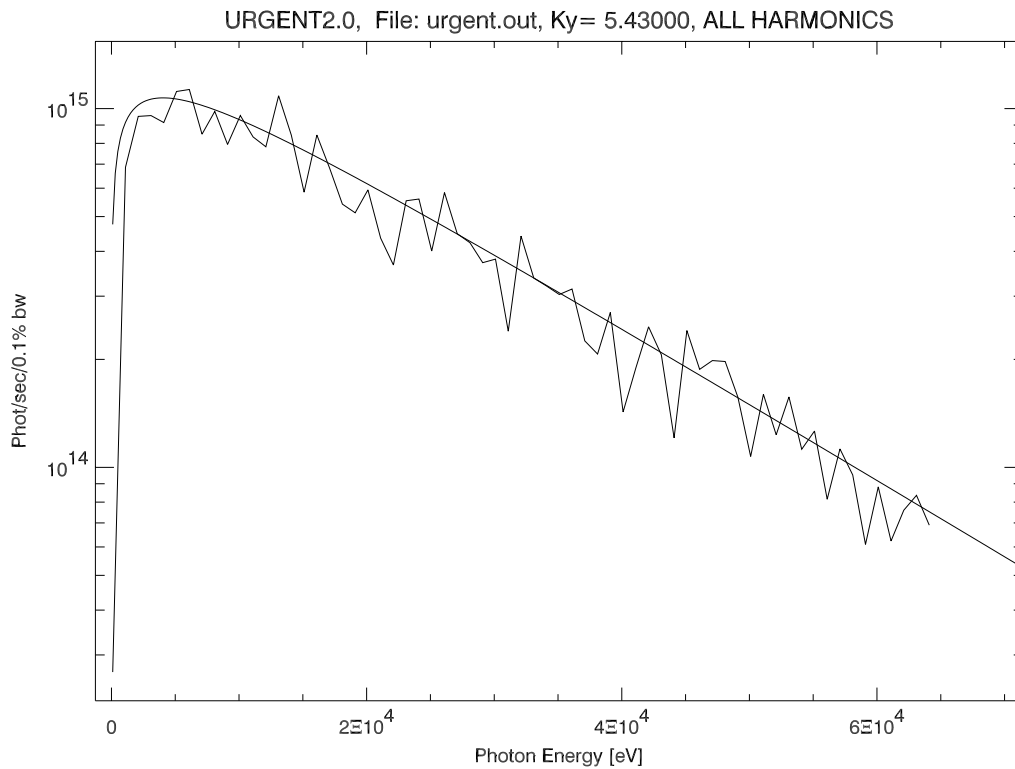
i) Use the files:

xurgent_id9_u20.

xurgent_id9_u46.xop

xurgent_id9_w70.xop

ii) For comparison, integrate over $1 \times 0.5 \text{ mrad}^2$:



6 – Filters and mirrors: effect on source

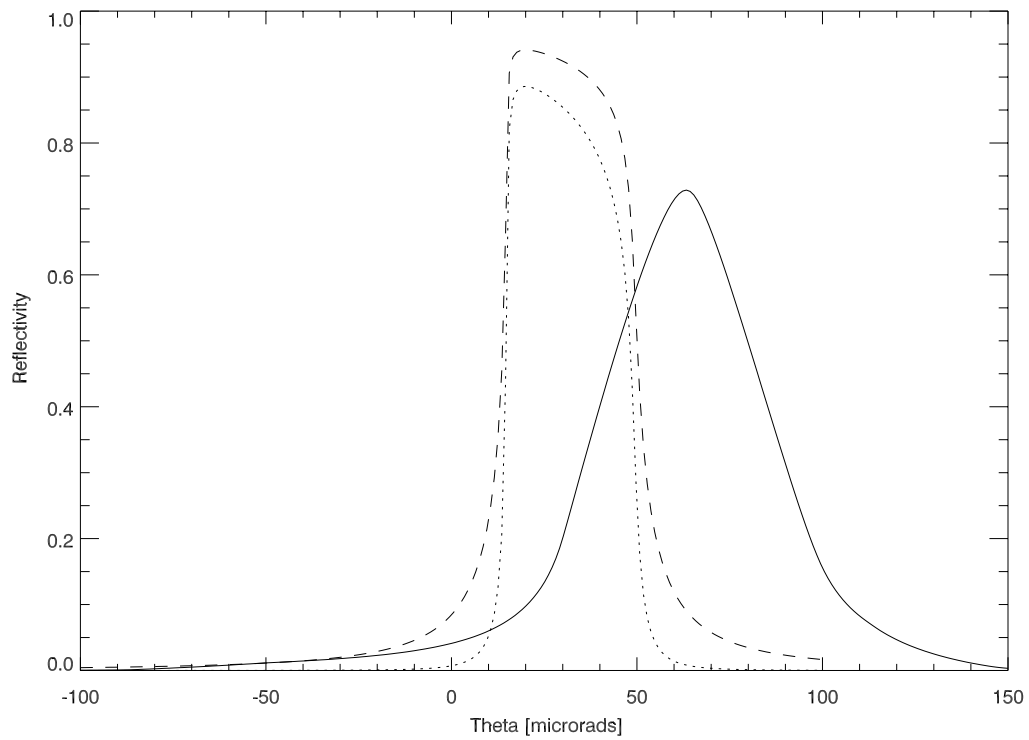
use the XOP input file xpower .xop

7 – Crystal monochromators

i)

Crystal	E [keV]	θ_B [deg]	W[μ 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



iii)

Si333 single reflection: $W=3.1$, $P=0.99$, $I=3.45 \Rightarrow$ Shifting $3.5 \mu\text{rad}$

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

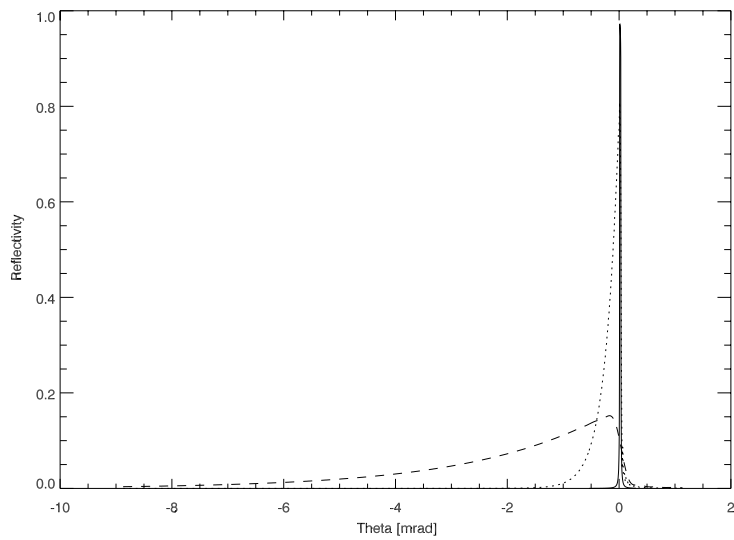
Si111.Si111: $W=33.8$, $P=0.88$, $I=29.2$

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

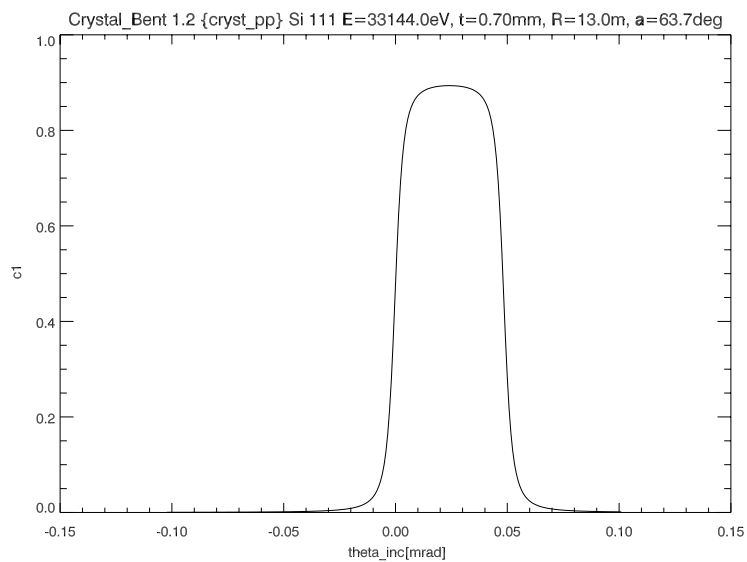
8 – Bent crystals

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

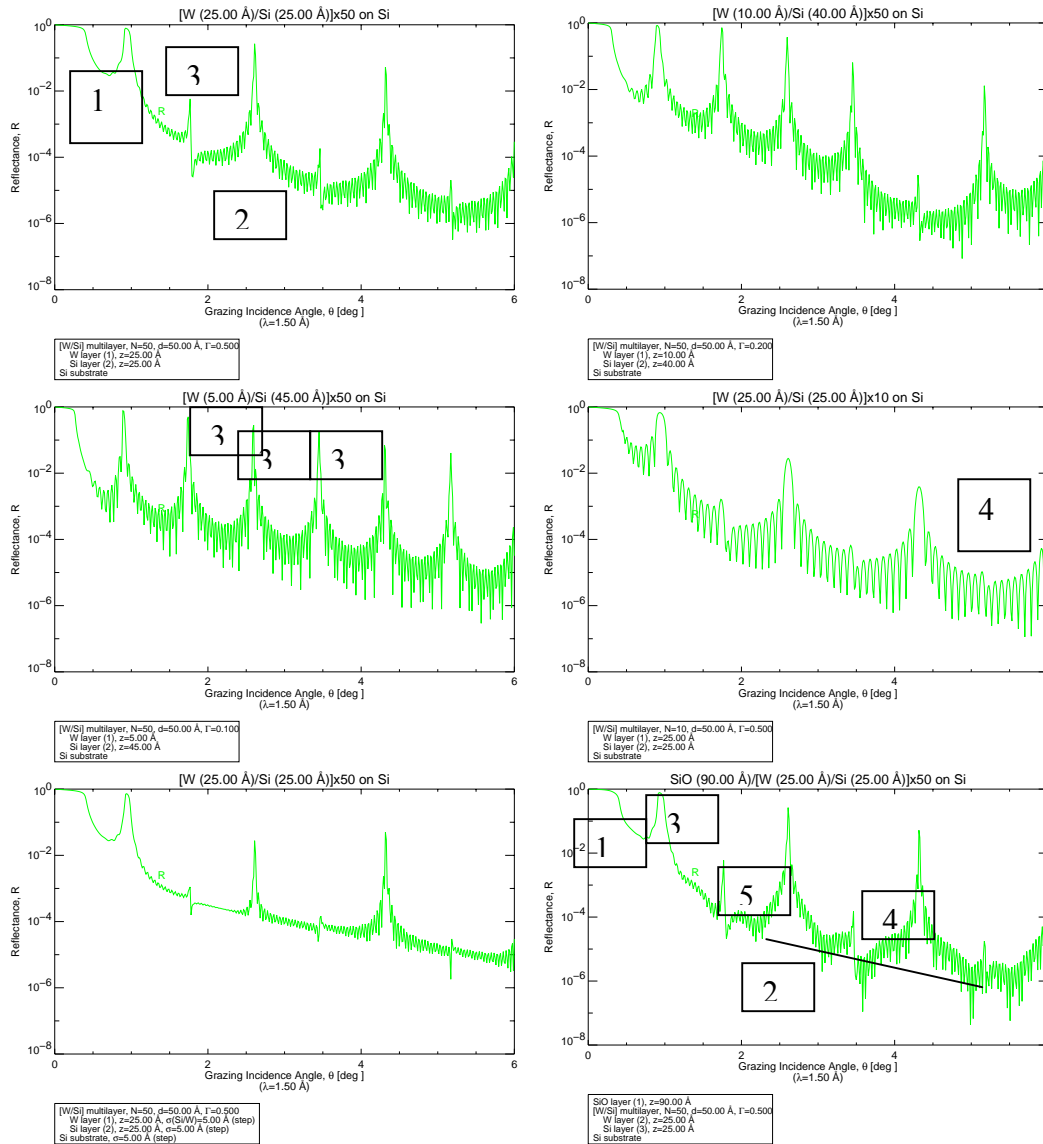


ii)



9 – Reflectivity curves of multilayers

- i) Use the file mlayer.xop
- ii) Start with the file 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.