XOP tutorial at ESRF - Session 4
Advanced ray-tracing

- Slope errors
- Thermal bump
- Curved crystal monochromators: Rowland and off-Rowland configurations
- Crystals in Laue geometry
- Macros: loops, grid-patterns, ad-hoc ray-tracing and post-processing.

- Appendix – focusing formulas for asymmetric crystals

- Answers

1. Slope errors.

You will learn to:

- Use `waviness_gen` to create a file sampling slope errors
- Use `presurface` to inject it in SHADOW
- See the important effect of slope errors in the focal size

a) Load the Kirkpatrick-Baez system of session 3 (exercise 6). Set mirror surface to be elliptical. Check that mirror dimensions are 40×4 cm^2 . Calculate spot sizes without slope errors.

b) use the program `waviness_gen` to create maps of slope errors:

- i) Run from a DOS shell `waviness_gen < wav_test1.inp` to create a slope of 0.5 arcsec and visualize the resulting surface using `presurface,'wav_test1.dat'` from a macro window.
- ii) Do the same with `wav_test2.dat` to obtain a rippled surface.
- iii) Use now the file `wav1.inp`. What are the slope error values?
- iv) modify the value of the initial Y slope error in order to get a value close to the desired tangential slope error of 0.5 arcsec rms. Then modify the number of points in X in order to adjust the sagittal slope error to 1 arcsec rms. Call the result `wav1opt.inp`. Create another file wav2opt.inp with the same inputs but changed the seed. Then visualize the resulting surfaces and run SHADOW's `presurface` for both surfaces (use for that a macro and type there `xsh_run,'presurface'`). Take as inputs `wav1opt.dat` and `wav1opt2.dat` and call the resulting files `wav1opt.sha` and `wav2opt.sha`, respectively.
- v) in SHADOWVUI oe menu, select modified surface: surface error…, and use then external spline with the corresponding *.sha file, one different file for each mirror to avoid coupled unphysical effects. Calculate then the spot size.

2. Thermal bump.

You will learn to:

- use a macro to create a file sampling a thermal bump
- use `presurface` to inject it in SHADOW
- see the effect of the bump in energy resolution.

Load the `session4_2.ws` workspace. Create the source. Run the macro to create a Gaussian bump. Run SHADOW's `presurface` with `bump.dat` to create y. Run the system (a single Si111 crystal) without and with thermal bump. See the changes in the energy resolution.

3. Curved crystal monochromators: Rowland and off-Rowland configurations

You will learn to:

- understand the effect of crystal radius in energy resolution and focusing conditions
- calculate the focusing conditions in and out Rowland configuration
- understand the importance of using contour curves with PlotXY

a) Using the same Gaussian source, verify the focusing conditions for a symmetrical Si111 Bragg crystal at 10 keV, with p=30m. Calculate ΔE. Calculate ΔE for R_t=5000 cm and R_t=2500 cm. Explain the differences.

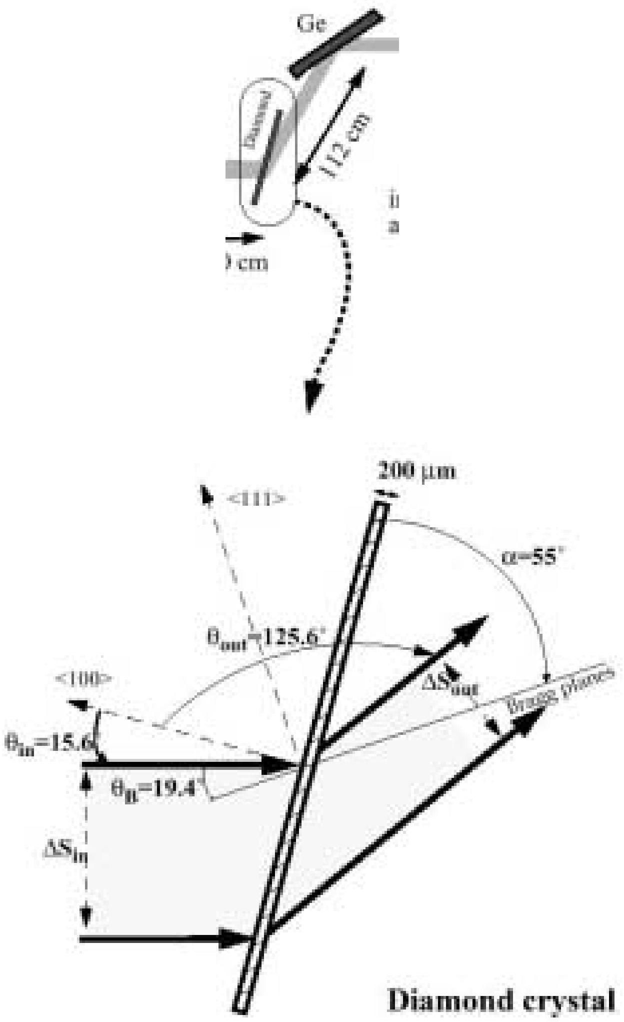
b) Calculate the Rowland conditions for 10 keV, Si111, p=30m and α=5º. Calculate energy resolution and spot size.

4. Crystals in Laue geometry

You will learn to:

- Set Laue crystals in SHADOW
- See the transformation in the phase space
- Apply a macro to copy intensity from one file to another.

Implement the system in file `session4_4.ws`, consisting in an asymmetric Laue diamond (111) crystal (a=3.55 Å) and a symmetric Bragg germanium (220) crystal (a=5.66 Å) in non-dispersive configuration. Notice that the diamond crystal has two associated screens, one before and another after it. Run the system, and then the macro that copies the electric vectors (i.e., intensities) from screen 2 to screen 1. Make histograms for these two screens and verify the changes in width for the z and z' coordinates. Relate these changes to the Liouville theorem.



5. Macros: loops, grid-patterns, ad-hoc ray-tracing and post-processing

Study the example SHADOWVUI workspaces in `C:\progra~1\xop2.0\extensions\shadowvui\workspaces`:

- `Ellipses_in_phase_s.ws` An example of grid source and presentation of its results using a macro
- `ESRF_bm5.ws`: shows how to run the source and the system from a macro
- `Loop.ws`: shows how to run shadow in a loop, and how to accumulate results.
- `Grid_pattern.ws`: shows how to trace grids with SHADOW using macros

Appendix Focusing formulas for asymmetric crystals (monochromatic beams)

Sagittal direction

$$\frac{1}{p}+\frac{1}{q}=\frac{\sin(\theta+\alpha)+\left|\sin(\theta-\alpha)\right|}{R_s} \quad (4.1)$$

Tangential or meridional direction

$$\frac{\sin^2\left(\theta+\alpha\right)}{p}+\frac{\sin^2\left(\theta-\alpha\right)}{q}=\frac{\sin(\theta+\alpha)+\left|\sin(\theta-\alpha)\right|}{R_t} \quad (4.2)$$

In the case of Bragg symmetrical crystals (a=0) they reduce to

$$\frac{1}{p}+\frac{1}{q}=\frac{2\sin\theta}{R_s};\quad \frac{1}{p}+\frac{1}{q}=\frac{2}{R_t\sin\theta}; \quad (4.3)$$

The Rowland condition (where the angular spread of the beam onto the Bragg planes is minimized, thus leading to the optimum energy resolution) is

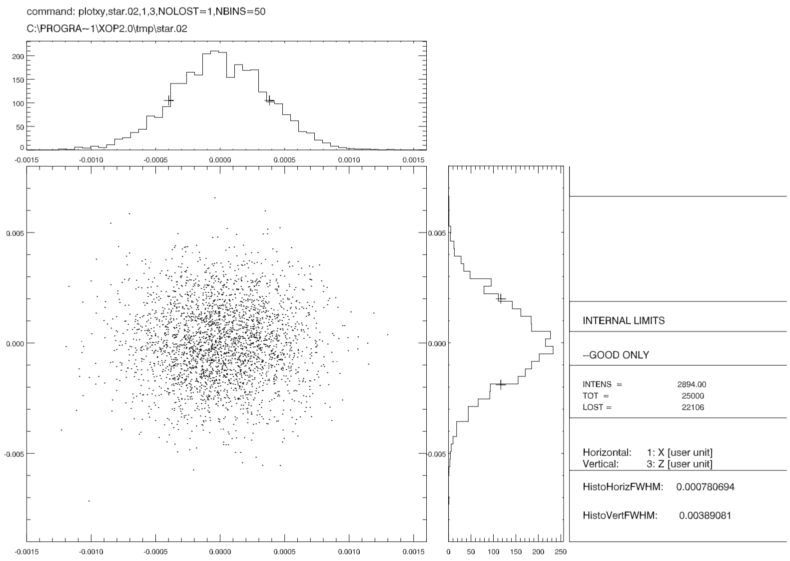
$$p=R\sin\left(\theta+\alpha\right) \quad (4.4)$$

In order to verify both the focusing equations and the Rowland condition for α=0, the condition p=q (magnification one) must be satisfied.

Answers

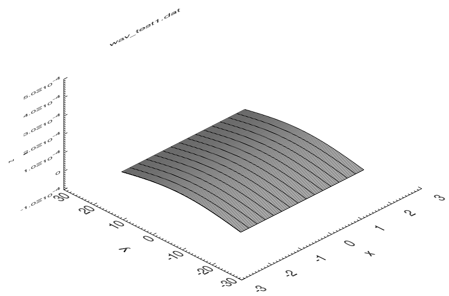
1 - Slope errors

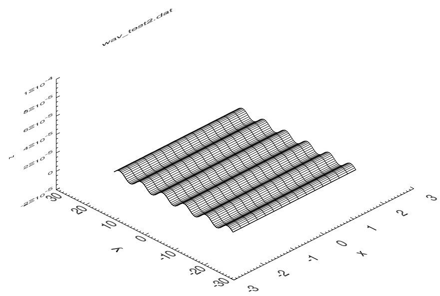
a) 8×40 μm^2



b)

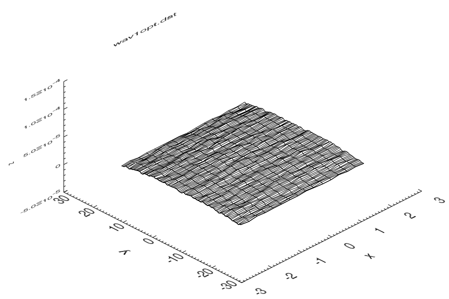
i) and ii)



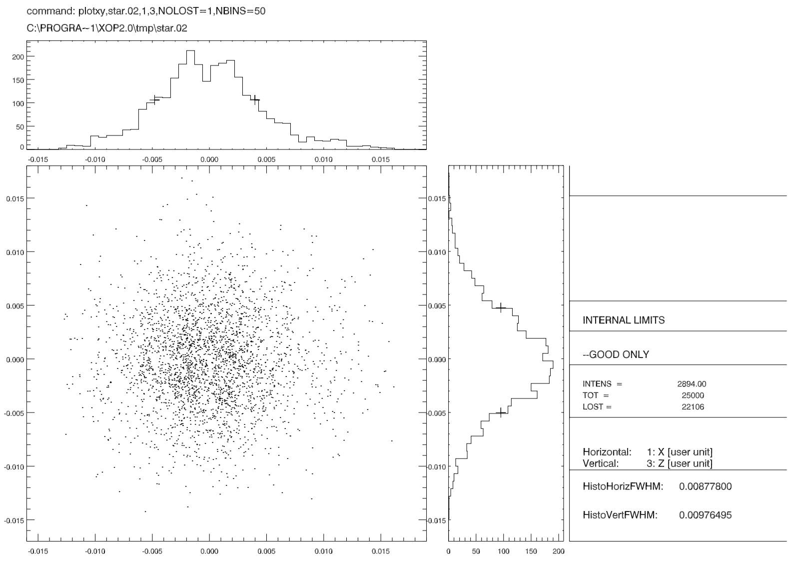


iii) 0.28 arcsec (Y) × 0.73 arcsec (X)

iv)

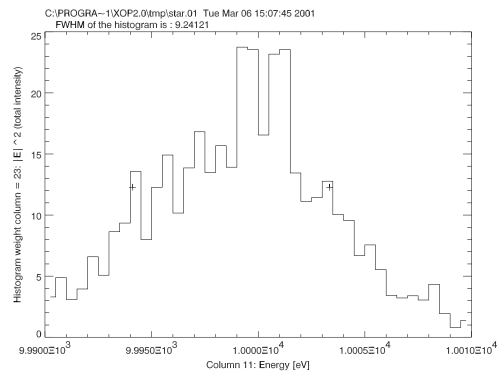


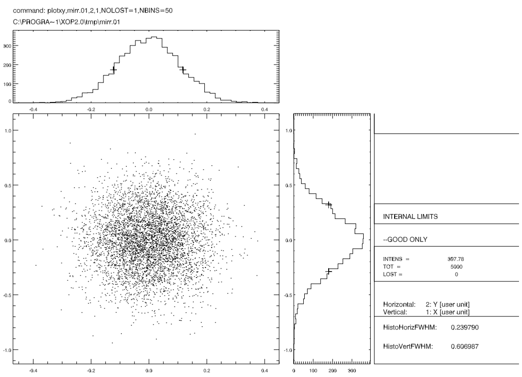
v) 88 × 98 μm^2



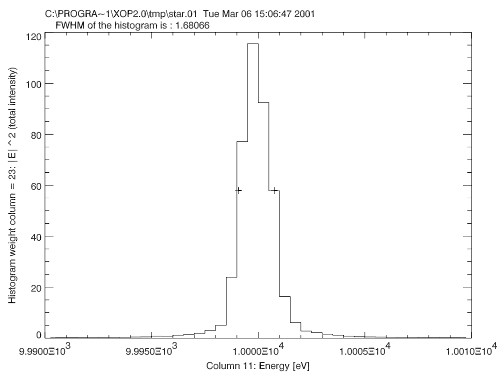
2 - Thermal bump

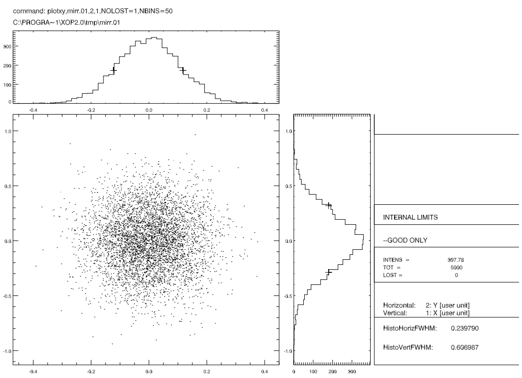
With bump:





Without bump





3 - Curved crystal monochromators: Rowland and off-Rowland configurations

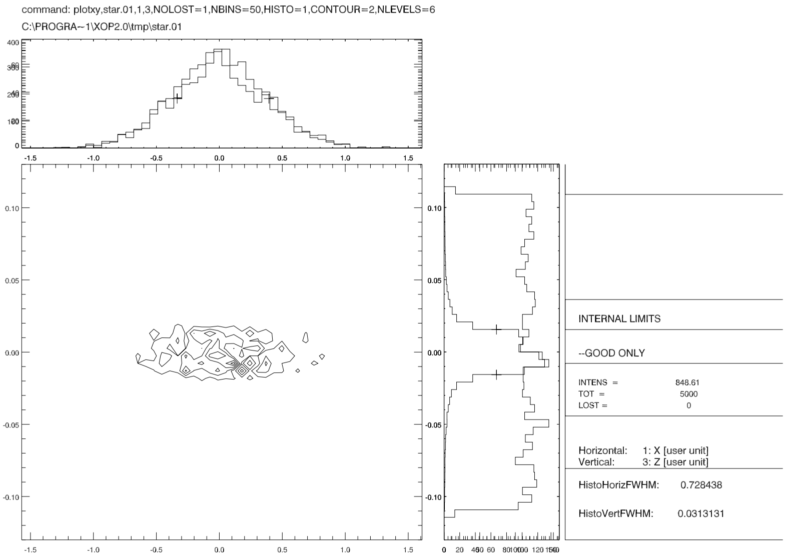
Answers

a)

R_t=15171 cm; ΔE=1.36 eV;

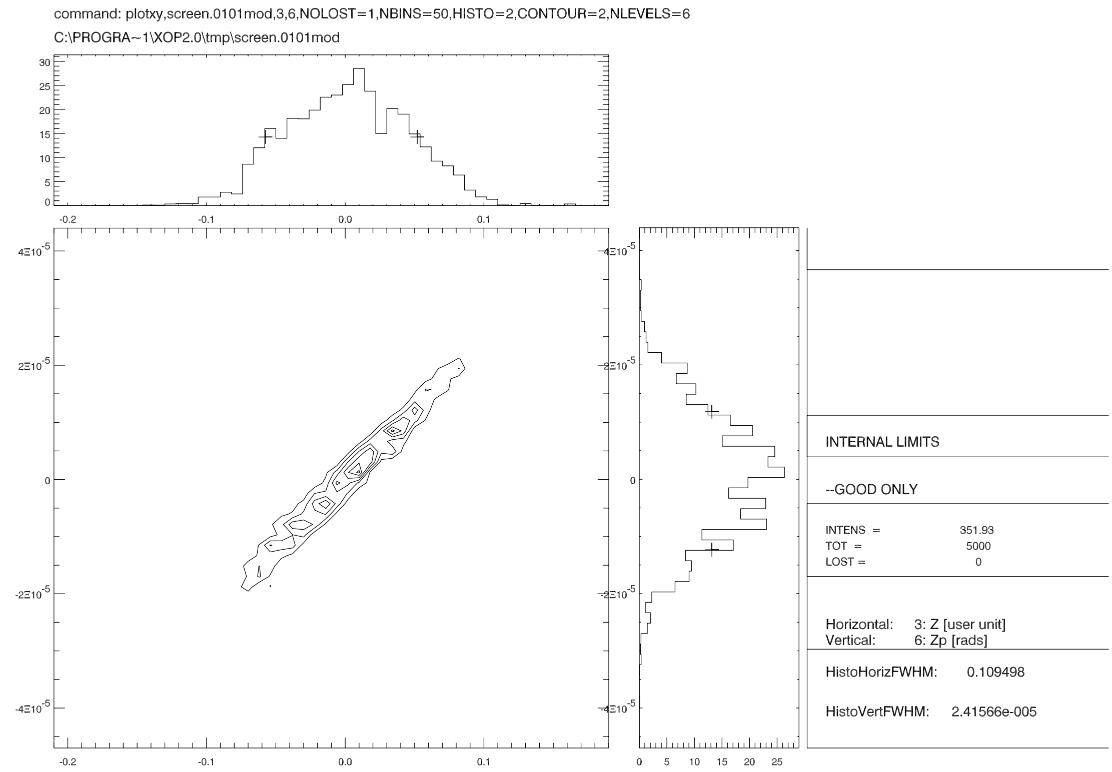
ΔE=2,3 eV, for R_t=5000, 2500 cm, respectively

b) R_t=10622 cm, q=1185 cm; .ΔE=0.85 eV; spot size = 0.77×0.033 cm^2.



4 - Crystals in Laue geometry

Before



After