Advances in phase space analysis of synchrotron radiation x-ray optics

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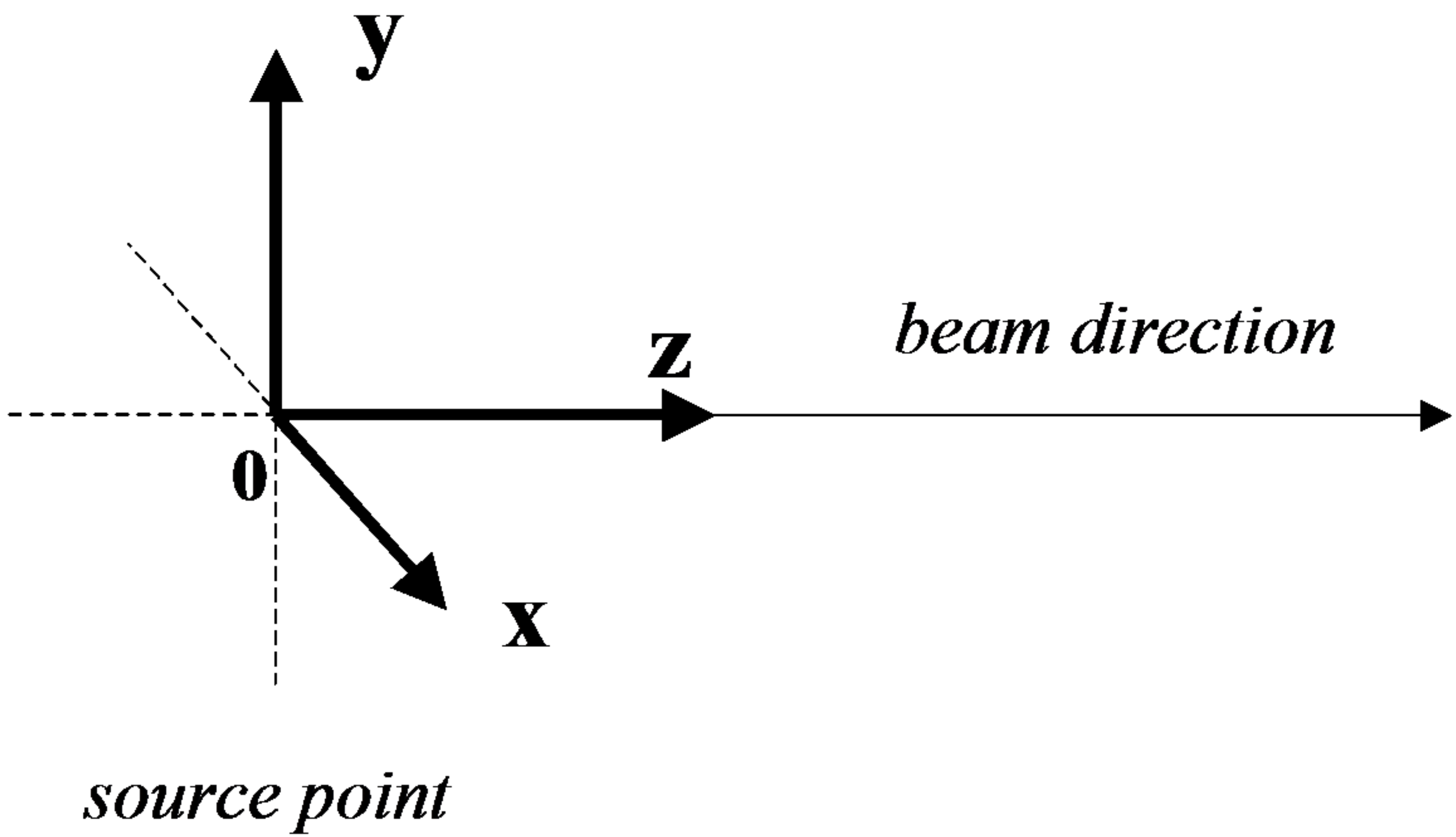


Coordinate system used to describe the beam propagation from the x-ray source through optics to sample

$$\begin{pmatrix} y_2 \\ y_2' \\ \Delta\lambda / \lambda \end{pmatrix} = \mathbf{A} \begin{pmatrix} y_1 \\ y_1' \\ \Delta\lambda / \lambda \end{pmatrix}$$

$$f_2(y_2, y_2', \Delta\lambda / \lambda) = f_1(y_1, y_1', \Delta\lambda / \lambda) = f_1[\mathbf{A}^{-1} \begin{pmatrix} y_2 \\ y_2' \\ \Delta\lambda / \lambda \end{pmatrix}]$$

$$\mathbf{y}_2 = \mathbf{T}_2 \mathbf{y}_3, \mathbf{y}_1 = \mathbf{T}_1 \mathbf{y}_2 \Rightarrow \mathbf{y}_1 = \mathbf{T}_1 \mathbf{T}_2 \mathbf{y}_3$$

where $\mathbf{T}_i$ are the inverse matrices of those usually given (Matsushita, Handbook of Synchrotron Radiation)

transformation matrix

flight path

$$\begin{bmatrix} 1 & -L & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

plane monochromator

$$\begin{bmatrix} b & 0 & 0 \\ 0 & \frac{1}{b} & (1-\frac{1}{b})\tan(\theta_B) \\ 0 & 0 & 1 \end{bmatrix}$$

curved monochromator

$$\begin{bmatrix} b & 0 & 0 \\ \frac{1}{f_c} & \frac{1}{b} & (1-\frac{1}{b})\tan(\theta_B) \\ 0 & 0 & 1 \end{bmatrix}$$

acceptance window

Source, transmission functions and acceptance windows are approximated by Gaussian functions

$$A(y', \frac{\Delta\lambda}{\lambda}) = 4\sqrt{\frac{2}{3\pi}} Exp\left(-\frac{\left(y' - \frac{\Delta\lambda}{\lambda}\tan\theta_B \right)^2}{2\sigma_D^2} \right) \qquad A(\lambda) = \sqrt{\frac{6}{\pi}} Exp\left(-\frac{\left(\frac{\Delta\lambda}{\lambda} \right)^2}{2\sigma_\lambda^2} \right)$$

$$W_D = \frac{W_S}{\sqrt{b}} \qquad \sigma_D^2 = \frac{W_D^2}{12} \qquad \sigma_\lambda^2 = (\sigma_{y'}^2 + \sigma_D^2)(\cot\theta_B)^2$$

$$A(y, y', \frac{\Delta\lambda}{\lambda}) = 4\sqrt{\frac{2}{3\pi}} Exp\left(-\frac{\left(y' - \frac{y}{R_c \sin(\theta_B + \alpha)} - \frac{\Delta\lambda}{\lambda}\tan\theta_B \right)^2}{2\sigma_D^2} \right) \qquad A(\lambda) = \sqrt{\frac{6}{\pi}} Exp\left(-\frac{\left(\frac{\Delta\lambda}{\lambda} \right)^2}{2\sigma_\lambda^2} \right)$$

$$\sigma_\lambda^2 = \sigma_D^2 (\cot\theta_B)^2$$

transformation matrix **acceptance window**

mirror

$$Exp\left(-\left(\frac{4\pi\sin(\Theta_i)\sigma_r}{\lambda_M}\right)^2\right)\begin{bmatrix}1 & 0 & 0\\ \frac{1}{f_m} & 1 & 0\\ 0 & 0 & 1\end{bmatrix}$$

cylindrically curved multilayer

$$\begin{bmatrix}1 & 0 & 0\\ \frac{1}{f_c} & 1 & 0\\ 0 & 0 & 1\end{bmatrix}$$

$$A(y,y',\frac{\Delta\lambda}{\lambda}) = \frac{8}{3}R_{ML}\sqrt{\frac{Ln(2)}{\pi}}Exp\left(-\frac{\left(y'-\frac{y}{R_c\sin\theta_{ML}}-\frac{\Delta\lambda}{\lambda}\tan\theta_{ML}\right)^2}{2\sigma_{ML}^2}\right)$$

$$\sigma_{ML} = W_{ML}/2\sqrt{2Ln(2)}$$

$$W_{ML} = 2\lambda\sqrt{Ln(2)/\pi} \;/\; Na\square\cos\vartheta_{ML}$$

$$\sigma_\lambda^2 = \sigma_{ML}^2(\cot\theta_{ML})^2$$

refractive lens with parabolic holes

$$\begin{bmatrix}1 & 0 & 0\\ \frac{1}{F} & 1 & 0\\ 0 & 0 & 1\end{bmatrix}$$

$$\frac{1}{F} = \frac{2N\delta}{R}$$

$$A(y) = Exp\left(-\frac{y^2+Rd}{2\Sigma^2}\right)$$

$$\Sigma^2 = \frac{\delta}{4\pi\beta+\lambda/l_s}\lambda F$$

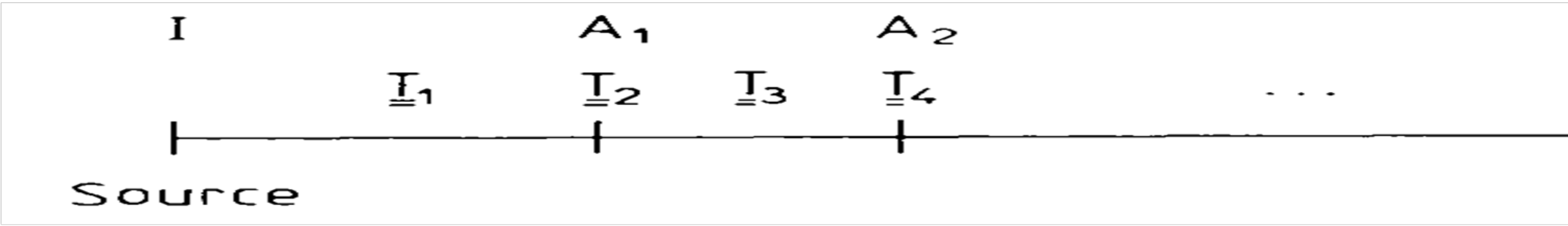
Source

$$I(x, x', y, y', \lambda) = I(0,0,0,0,\lambda) I_x(x, x') I_y(y, y') I_\lambda(\Delta\lambda / \lambda)$$

$$I_x(x,x') = \exp[-(x^2/\sigma_x^2 + x'^2/\sigma_{x'}^2)/2]$$

$$I_y(y,y') = \exp\{-[y^2/\sigma_y^2 + (y' - \Gamma y)^2/\sigma_{y'}^2]/2\}$$

$$I_\lambda(\Delta\lambda/\lambda) = \exp[-(\Delta\lambda/\lambda)^2/2\sigma_{s\lambda}^2],$$



The coordinate transformation from source to sample is

$$\mathbf{y}_1 = \mathbf{T}_1\mathbf{T}_2\mathbf{T}_3 \ldots \mathbf{T}_N\mathbf{y}_N$$

The acceptance windows of the components are given at the entrance side of the components. They have to be transformed into the sample position and it is therefore convenient to do the matrix multiplication from the right side to the left of the product.

$$I_{sample}(x, x', y, y', \Delta\lambda / \lambda) = IA_1 \ldots A_M R_1 \ldots R_k F$$

The total number of photons Φ at the sample position per second (the flux) is

$$\Phi = \int I_{sample} dx dx' dy dy' d(\Delta\lambda / \lambda)$$

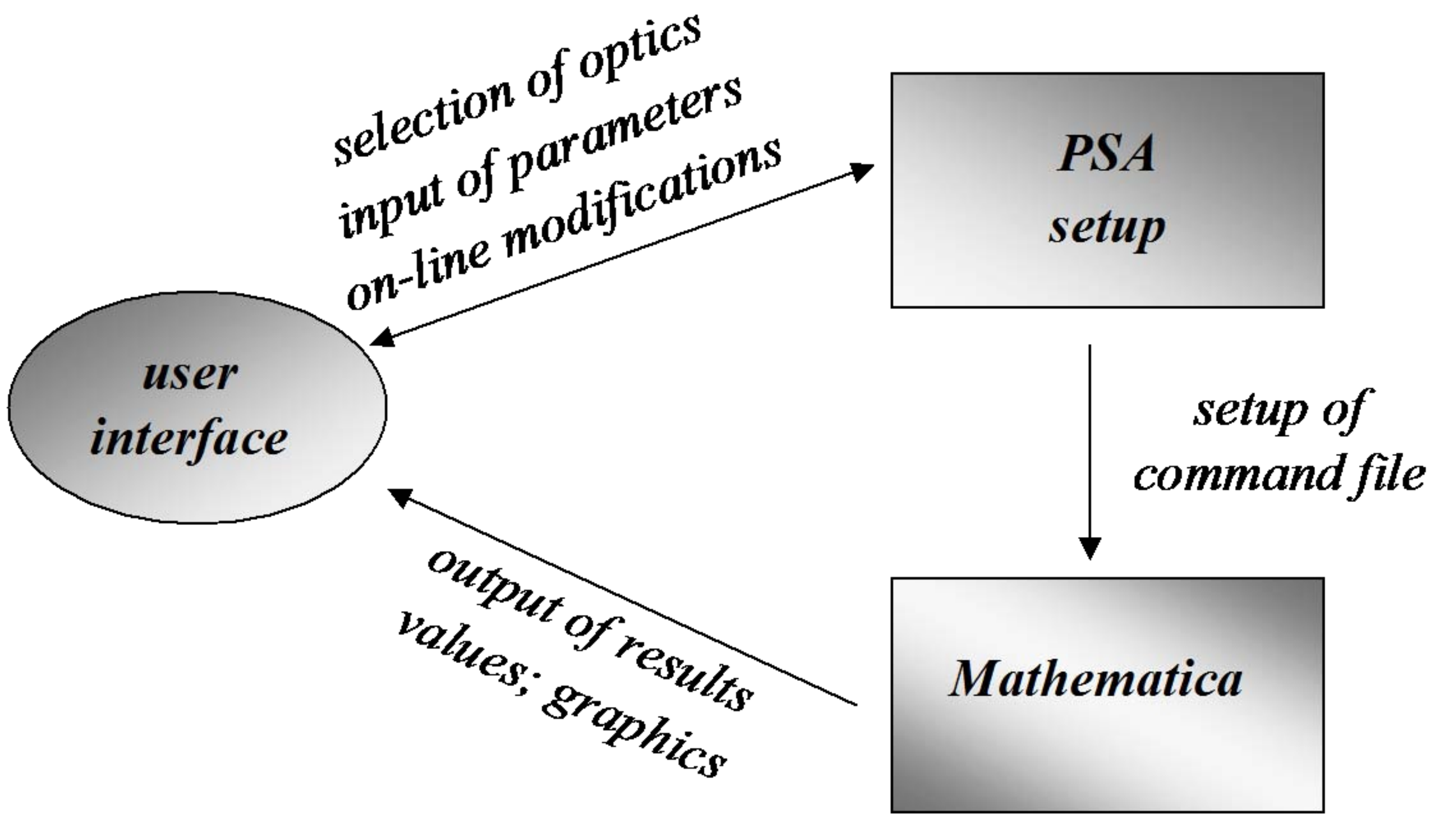
The general form for the intensity distribution at the sample position is:

$$I_{sample} = K_0 I_x(x, x') I_y(y, y', \Delta\lambda / \lambda)$$

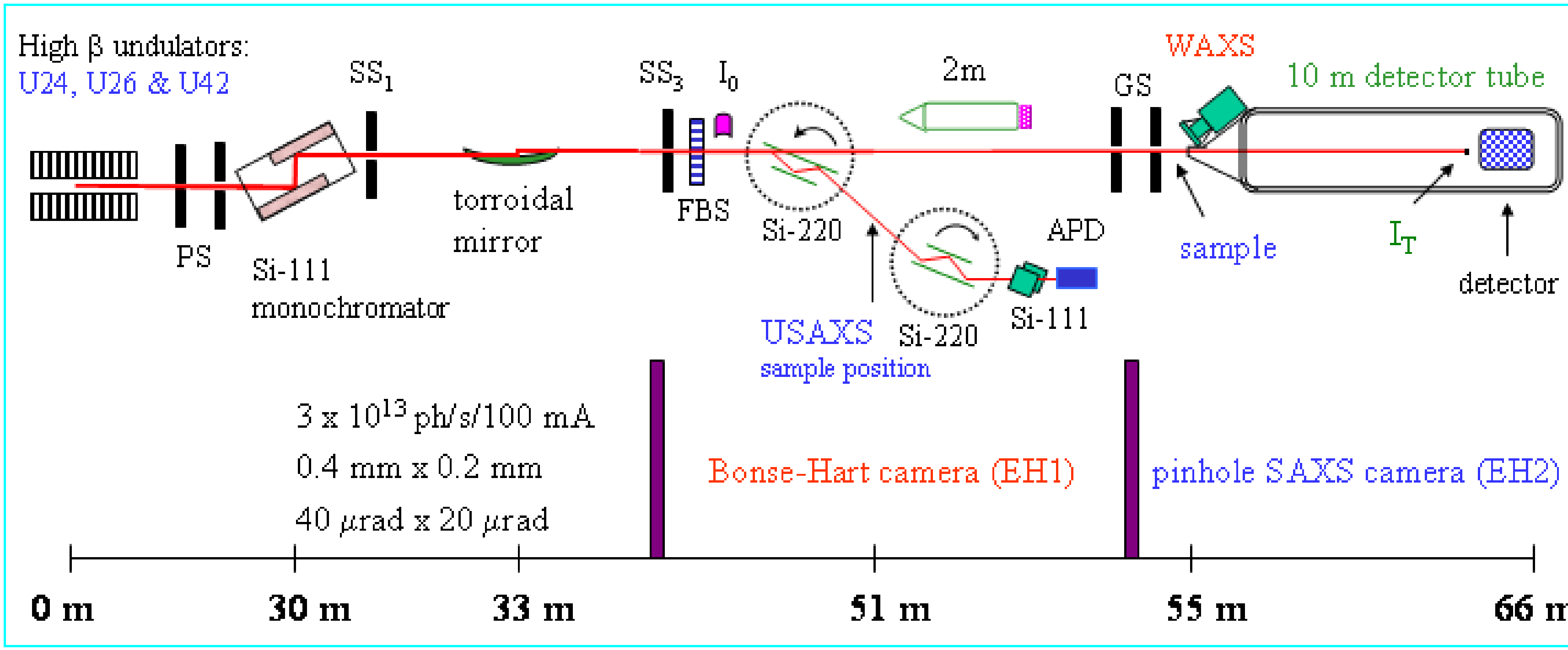
we assume the distribution of photons in position-angle space in the vertical and horizontal direction to be independent. This is an assumption usually used in beamline analysis. Due to this the transformations can be described by 3 x 3 matrices for position-angle-wavelength in the scattering plane of the monochromator crystals and 2 x 2 matrices for position-angle in the perpendicular plane. The spatial distribution of the beam can be calculated by integration of the wavelength and angle parameters:

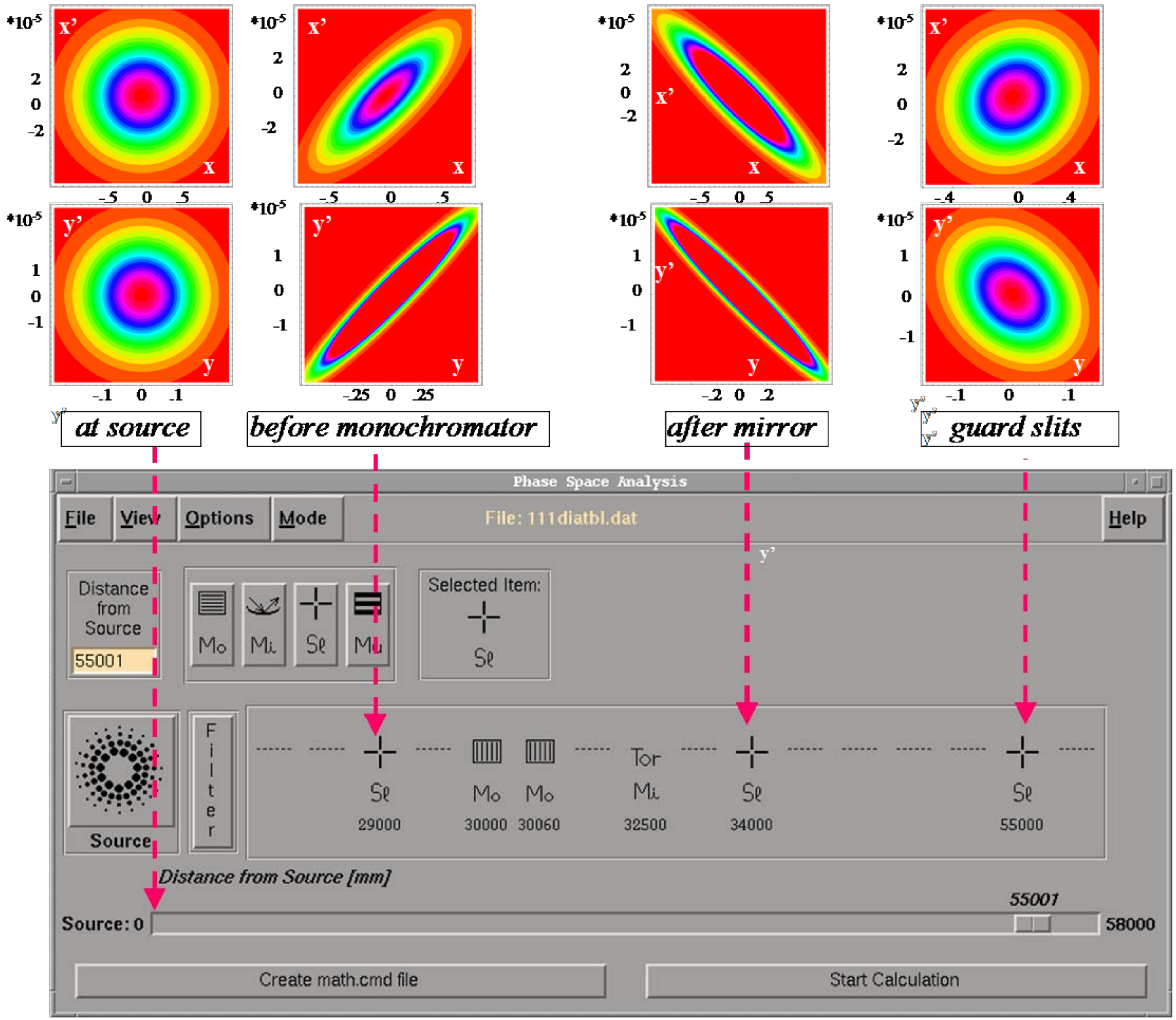
$$I(x,y) = K_0 \int I_y(y,y',\Delta\lambda/\lambda) I_x(x,x') \mathrm{d}(\Delta\lambda/\lambda) \mathrm{d}y' \mathrm{d}x'$$

Schematic design of the PSA computing toolbox

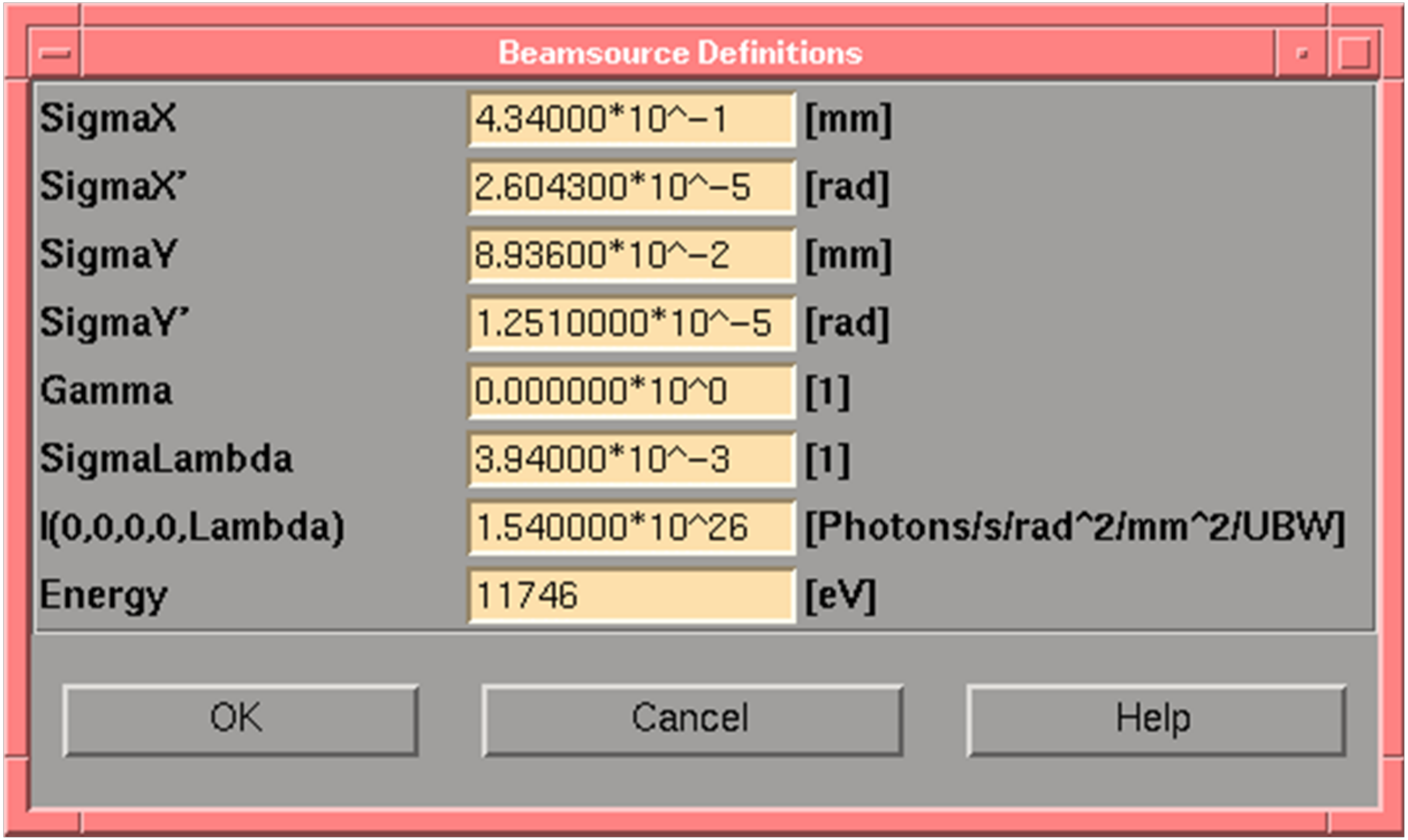


Schematic design of the ID02 beamline at the ESRF





Graphical user interface (GUI) showing a selection of optical components for the ID2 SAXS beamline. Phase space diagrams were calculated by PSA. Note the change of scales between different PS-diagrams. (units: x,y: mm; x',y':Rad)

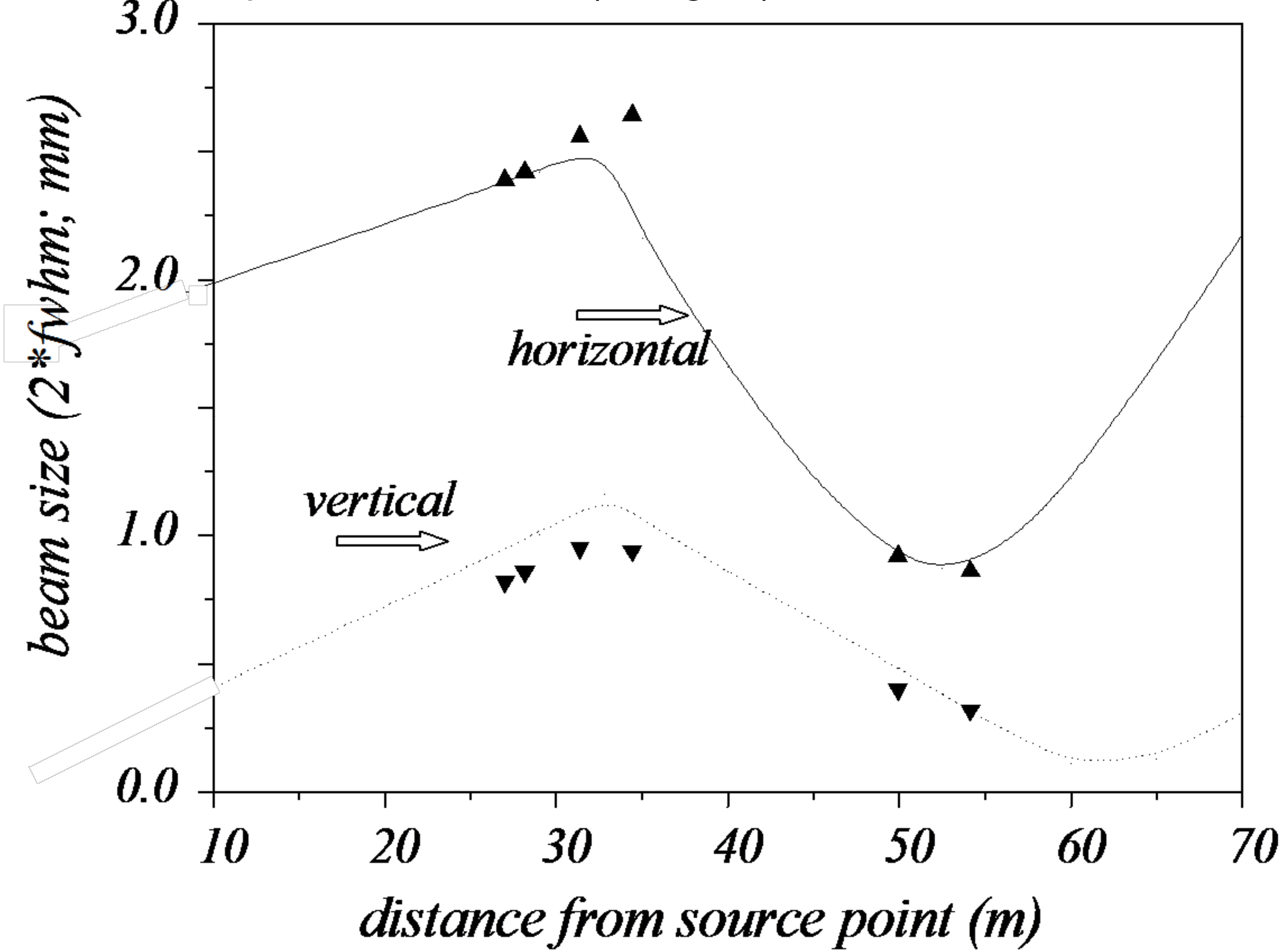


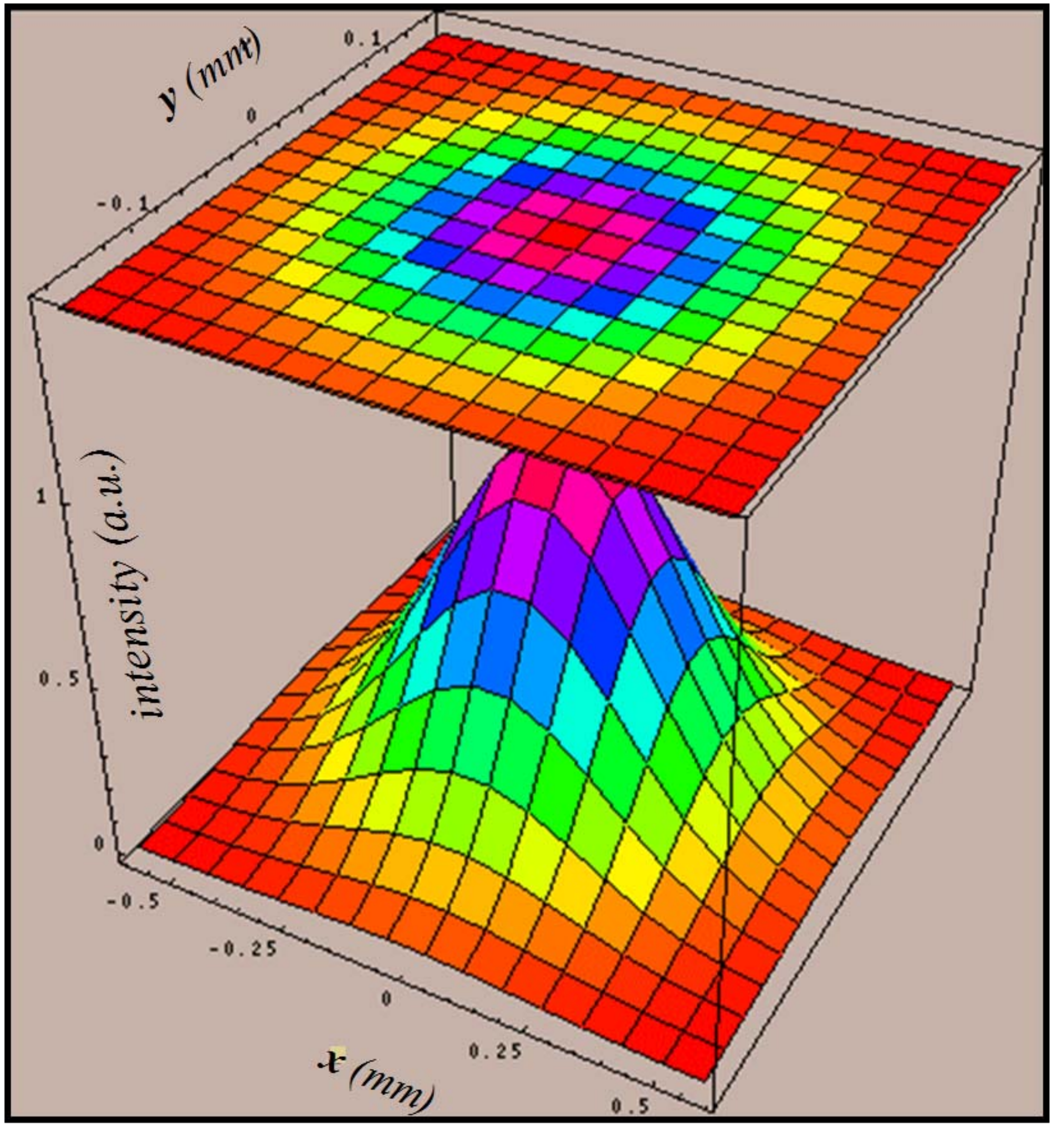
ID2 undulator input parameters in the GUI icon

Comparison of phase space analysis (PSA) and ray-tracing (SHADOW) results of the ID02 beamline

Optical Element		Flux	x (fwhm)	y (fwhm)	x' (fwhm)	y' (fwhm)	$\Delta\lambda/\lambda$ (fwhm)
		*ph/s[10^{13}]	[mm]	[mm]	[μrad]	[μrad]	*[10^{-3}]
Source	**PSA**	2,615	1,02	0,21	61,3	29,5	9,28
	SHADOW	2,618	1,02	0,21	61,2	29,4	
Slit 1	**PSA**	2,134	1,49	0,68	49,3	23,3	9,28
	SHADOW	2,373	1,55	0,73	48,0	24,5	
Si-111 Mono	**PSA**	0,807	1,53	0,65	49,3	19,6	0,128
	SHADOW	0,877	1,59	0,74	47,8	23,8	
Mirror	**PSA**	0,807	1,63	0,69	66,0	25,0	0,128
	SHADOW	0,859	1,69	0,80	70,4	26,8	
Slit 2	**PSA**	0,782	1,26	0,54	56,5	20,9	0,117
	SHADOW	0,822	1,50	0,69	69,5	25,0	
Slit 3	**PSA**	0,782	0,53	0,17	56,3	20,6	0,111
	SHADOW	0,799	0,55	0,22	69,7	24,7	

Comparison of beam sizes in horizontal and vertical direction, respectively, calculated by PSA (lines) and experimental values (triangles) for the ID02 beamline.





Intensity distribution calculated at 55 m from the source point (guard slits of SAXS end station)