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R A Y

THE BESSY RAYTRACE PROGRAM

to calculate

SYNCHROTRON RADIATION BEAMLINES

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                 THE BESSY RAYTRACE PROGRAM

                 Version 24.4 of JAN 4, 2006

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H I S T O R Y

NEWS:- RAY_SOU, RAY_TRA, RAY_OUT for ellipsoids on PDP11 Nov. 84
- RAY Version 1.0 on VAX (Jupp's special) Dec. 85
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- Michael's Quartz-crystal special 20. 3.96
- Gerd's trapezoidal grating special 24.12.97
- Diffraction effects on SL_its 28. 7.98
- SGM fix-focus option (Fred special) 25. 2.99
- asymmetric – gradient Cylindrical crystal option CC 21. 3.00
- accepting Multilayers on all optics (Franz special) 3. 4.00
- accepting Stokes vector from WAVE-input 14. 4.00
- accepting ANSYS-profiles (Olaf special) 19. 4.00
- Central beamstop at SL_its (Bill's IR-special) 9. 5.00
- Including rotation sense f. DI_pole 16. 5.00
- Laterally graded multilayers (Alexei special) 29. 9.00
- Array for surface profile set to 251 x 251 pixels 14. 6.01
- RAY Version for PC-Windows available (Dirk special) 15. 3.02
- Elliptical toroid (high-order diaboloid)(Gerd special) 13. 8.02
- Testversion for ZO_neplates- Nikolay special 21.3.03
- Source pathlength included 1.10.03
- Raman scattering - Rolf special 6.09.04
- Energy distribution data file - Rolf special 16.12.04
- Testversion for Reflection Zoneplates (RZ) 10.02.05
- The WAVEFRONT version 12.05.05
- The REAL and FINAL EXPERTS-OPTICS version 8.12.05

ABSTRACT

The raytracing program *RAY* simulates the imaging properties of an optical system. It randomly creates a set of rays within various types of light sources and traces them according to the laws of geometric optics through optical elements onto image planes. The distribution of the rays at the source, optical elements and image planes can be displayed.

A ray is described not only by its coordinates with respect to a suitable coordinate system, but also by its energy and its polarisation determined by the Stokes vector.

Different source types are implemented with special emphasis on a realistic simulation of source intensity, volume and emission characteristics, especially for synchrotron radiation (dipole- and undulator-) sources. Optical elements can be reflection mirrors of nearly any figure (plane, cylindrical, spherical, aspherical...), gratings, zone plates, foils or crystals. The absolute transmission of the optics including the effect of optical coatings is calculated according to the reflection/refraction/transmission process from the optical constants of the involved materials. The influence of misalignment of the source and/or the optical elements, slope errors and thermal deformation of the optics can also be taken into account. A graphic display of spot patterns at any position of the beam, intensity and angular distributions, absolute flux, polarisation, energy resolution is possible.

CONTENTS

1. Introduction

The development of the raytracing program *RAY* was started at BESSY in 1984 for basic raytracing calculations of VUV- and soft x-ray optical schemes /1/. Since that time *RAY* has been in continuous evolution and it has grown into a widely used design tool for synchrotron radiation beamlines as well as for other optical systems. Most of the BESSY I monochromators have been designed with *RAY*. In order to meet the requirements of the new undulator-based third generation storage ring BESSY II, many new features have been implemented into the code. such that *RAY* now has become an indispensable tool for modern beamline design. It’s capabilities are similar to the widely used *SHADOW* program /2/. Considerable effort has been made to ensure that it is a a user friendly, easy accessable and easy-to-learn program for everyday use with a minimum effort on data- and file handling.

Alternatively to these programs based on *intensity* distributions and on geometric optics the program *PHASE* has been developed /3/ which on the basis of complex electric field distributions of synchrotron radiation sources is able to intrinsically take into account interference effects.

Some copies of *RAY* have been distributed to other laboratories and institutions, but the prefered present day’s use is to run the most actual BESSY-version worldwide interactively via a computer network from any account on the BESSY computer system. This avoids updatings and uncontrolled proliferation of older versions which makes the maintainance of the code impossible.

This report is intended to be a quick and practical reference and to give examples for the use of the program rather than to give a detailed outline of the underlying geometrical, mathematical, physical and optical principles which can be found in textbooks like /4-7/ or synchrotron radiation handbooks /8,9/. In particular the chapter 3.2 of reference 9 (Ray tracing) is strongly recommended as an introductory guide before calculating a real beamline design. Here the procedure, problems, limitations and the importance of *checking* the raytrace results for the various kinds of errors that can occur are discussed. Various specific *RAY*-features have been described in /10-14/. Examples for the use of the program in a variety of applications are given in /15-20/.

2. General

The raytracing program *RAY* simulates the imaging and focussing properties of an optical system. It randomly creates a set of rays within various types of light sources and traces them through one or more optical elements onto image planes. The geometric distribution of the rays at the source, all optical elements and the image planes can be visualized.

Various interesting features like focal properties, power distribution, energy resolution, rocking curves, absolute transmission and polarization characteristics of an optical setup are simulated. It combines the pure geometrical raytracing with calculations of the absolute transmission and is, thus, a central and indispensable part of the BESSY software tools for the design and optimization of new VUV- and x-ray monochromators and beamlines. The interplay of the software tools available at BESSY is demonstrated in Fig. 1 as a flowchart.

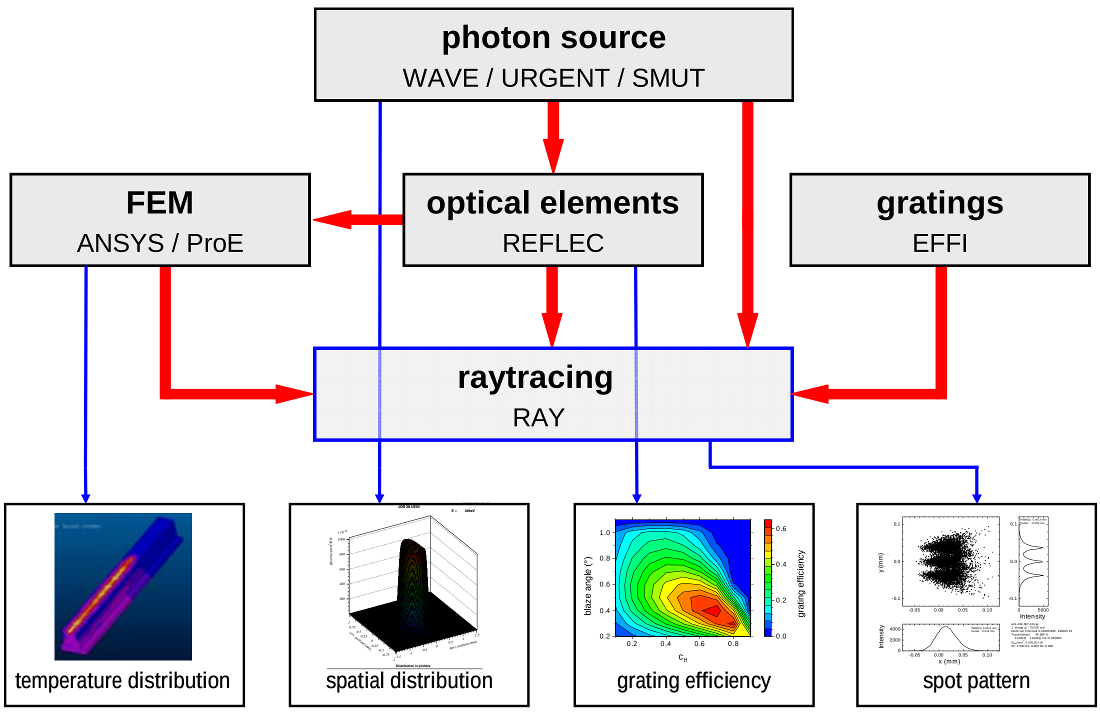

Figure 1 BESSY soft x-ray computational tools and their interplay (see references 13, 21-26)

Special emphasis was put on realistic simulations of (especially synchrotron radiation) beamlines: the path of the photons can be followed from any source including bending magnets and insertion devices via reflection/diffraction/transmission at optical elements through apertures, entrance and/or exit slits onto the sample. The influence of slope errors, surface roughness, thermal bumps, measured or calculated surface profiles as well as a misalignment of the source and optical elements can be studied in a simple way. Thus, it is possible to predict the real performance of the beamline under realistic conditions and to specify the requirements for all the components to be ordered.

In a well defined source volume, rays are created within a given horizontal and vertical divergence. Different source types have been implemented with special emphasis on a realistic simulation of the source including e.g. electron beam emittance effects. Each ray has the same intrinsic probability. The spatial and angular intensity *distribution* of the source is given by the spatial and angular *density* of the rays (i.e. rays per volume and solid angle). Thus the outgoing rays simulate the intensity distribution of the corresponding source. The rays are traced according to geometrical optics through one or more optical elements (mirrors, gratings, foils, crystals, slits, zoneplates) of which the surface can have nearly any figure like plane, cylindrical, spherical, toroidal, paraboloidal or ellipsoidal and which can be arranged in any geometry (horizontal, vertical, oblique). Coma-corrected varied line spacing gratings and (graded) crystals with automatic calculation of structure factors can also be handled.

A ray is determined not only by its coordinates with respect to a suitable coordinate system (e.g. by it's starting point), and by it's direction with respect to this coordinate system, but also by its energy E, its polarisation, described by the Stokes vector $\vec{S}$ (S_0,S_1,S_2,S_3) and its pathlength. Thus, a ray is described by 12 parameters, which are traced through the optical setup and for which the modifications (the geometric and intensity modulation) are calculated according to its interaction with the optical coating (reflection/refraction/transmission). Since all rays have equal probability, (the intensity of a ray, S_0, is either *1* or *0*) the throughput of a beamline is simply given by the number of rays, for realistic sources multiplied with the absolute photon flux as scaling factor.
For a first overview of the focal properties of an optical system the horizontal and vertical width of the beam can be visualized along the beam path for determination of the focus position. At any position in the beam image planes can be defined. The footprints of the rays on the optical elements and the focal properties of the optical system are analyzed and are visualized graphically as point diagrams, *2-D* or *3-D* intensity distributions, contour plots, etc.

The menu-driven program is user friendly so that a first performance test of an optical design can be gained rapidly without any file handling. Once the beamline has been defined the parameters are stored and can be modified in a subsequent run. The graphics output is directed to monitors, postscript printers, but also postscript files or ASCII-tables of all results can be created.
A flowchart of the program is shown in Fig. 2.

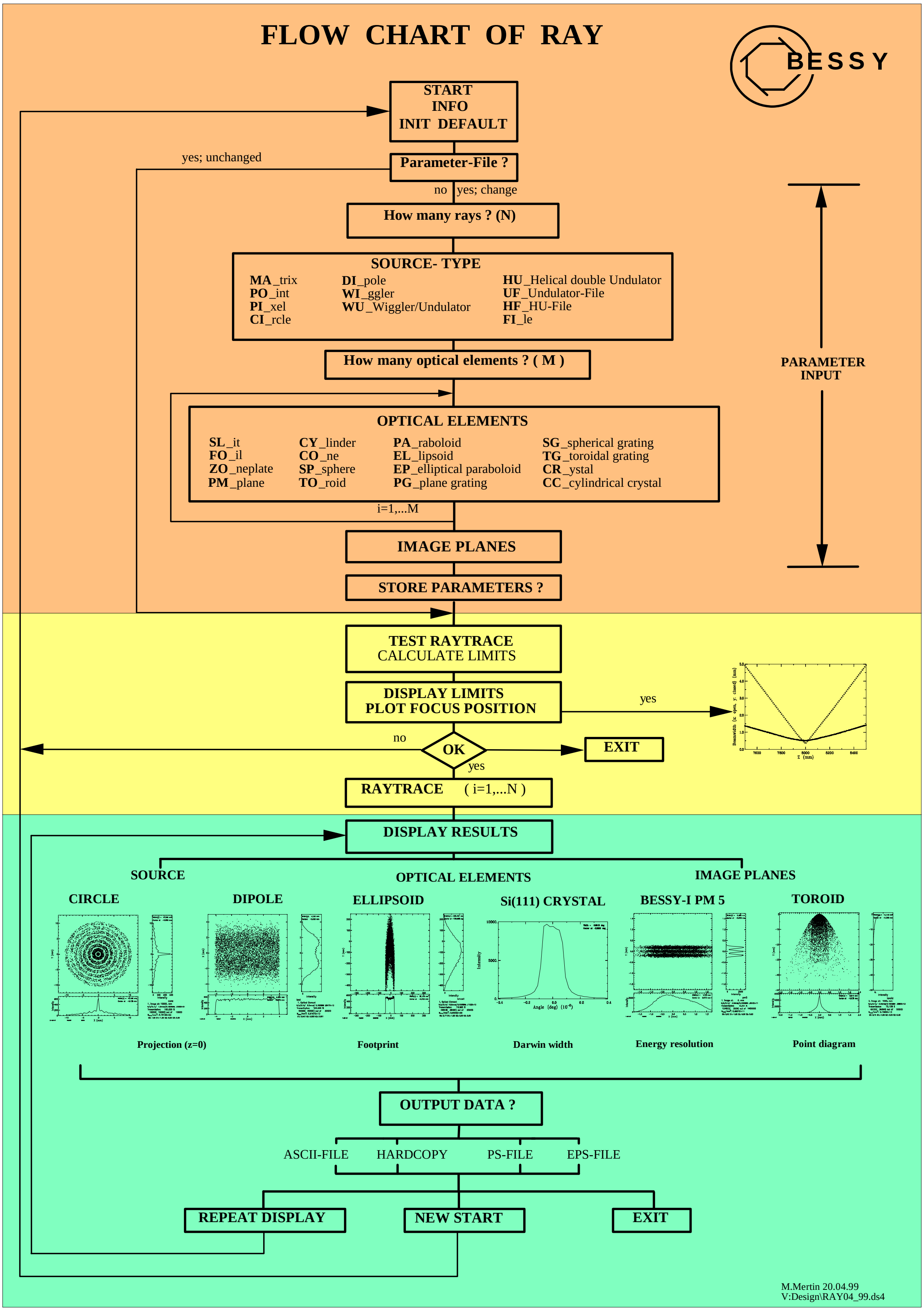

Figure 2 Flowchart of RAY

3. Theory

3.1 Statistics

To simulated realistic intensity patterns at optical elements and image planes (e.g. for heat load studies) it is necessary to create the source points and the rays in such a way that the same intensity is attributed to each ray.

Generally there are two possibilities:

1) A *systematic* distribution of the rays within the source so that the real emission characteristic is simulated. For this a large number of rays are required and need to be calculated before an optical setup is completely described.

2) The rays are distributed *statistically* within the source so that within the statistical error the real emission characteristic is simulated. The intensity distribution of the source is thus understood as probability distribution of all necessary parameters, namely position and angle. The main advantages of this Monto-Carlo procedure are its simplicity and the fact that a calculation of relatively few rays is already enough to create a reasonable simulation of the optics. When the statistics and the accuracy seem to be sufficient the calculation can always be interrupted without making a systematic error.

This second option is realized in *RAY. T*he procedure is as follows:

1) create a random number ran_1 between 0 and 1

2) scale the corresponding variable, e.g. the x-coordinate of the source point:

$$x = (ran_1 - 0.5) \bullet dx \qquad (1)$$

dx: source-dimension in x-direction

3) calculate the probability w of this randomly chosen start value for x (normalized to a maximum value of 1). E.g. the electron density in the Dipole-source (Gaussian profile $w(x)=exp(-x^2/(2\sigma_y^2))$ or the synchrotron radiation intensity for a fixed wavelength at a definite horizontal and vertical emission angle (Schwinger theory).

4) create a second random number ran_2. The ray is accepted only if the difference of the probability $w(x)$ and this new random number is larger than zero:

$$w(x) - ran_2 > 0 \qquad (2)$$

5) if the difference is less than zero neglect this ray and start again with a new one according to (1)

3.2 Sources

Various light sources are incorporated in *RAY*. Generally the rays are starting in a defined source volume and are emitted with a defined horizontal and vertical divergence. Either hard edges or a gaussian distribution profile can be selected. In the latter case rays are created statistically (see 3.1) within a +/-3σ-width of the gaussian profile (i.e. more than 99.9 % of the intensity).
For synchrotron radiation beamlines the polarised emission characteristic of bending magnets, wigglers and undulators are incorporated. For more complicated sources (like twin or helical undulators) or to take beam emittance effects into account the input can be given as an ASCII-file taken from programs for undulator radiation like *URGENT* /21/, *SMUT* /22/ or *WAVE* /23/. In this file the intensity and polarisation pattern of the light source must be described as intensity (photons/sec) and Stokes parameters at a distance of 10 m from the center of the source in a suitable *x-y* mesh. The file-structure is explained in Appendix A5.

Each ray is attributed an energy, *E,* and a polarization. The energy can be varied continuously within a „white“ hard-edge band of E_0+/-ΔE, or toggled between 3 discrete energies E_0, $E_0+\Delta E$ and $E_0-\Delta E$. This feature allows one to determine easily the energy dispersion and the spatial separation of discrete energies for monochromator systems, thereby giving a clear picture of the energy resolution one can expect.

The table 1 lists the main features of the different light sources implemented.

Source	**Matrix**	**Point**	**Pixel**	**Circle**	**Dipole**	**Wiggler**	**Wiggler/ Undulator**	**double Undulator (=2·PO)**	**Single Undulator ASCII-File**	**Helical Undulator ASCII-File**	**Source-Data File**
Name	**MA**	**PO**	**PI**	**CI**	**DI**	**WI**	**WU**	**HU**	**UF**	**HF**	**FI**
Width x	hard	hard/soft	hard	hard	soft	soft	soft	soft	soft	soft	soft
Height y	hard	hard/soft	hard	hard	soft	soft	soft	soft	soft	soft	soft
Length z	hard	hard	hard	hard	hard	$L=n\lambda_u$	0	hard	hard	hard	hard
Diverg. hor. ϕ	hard	hard/soft	hard	hard	hard	hard	calc.	soft	file	file	file
Diverg. vert. ψ	hard	hard/soft	hard	hard	calc.	calc.	calc.	soft	file	file	file
Stokes-Par. S_0	1	1	1	1	flux/s	flux/s	flux/s	flux/s	flux/s	flux/s	flux/s
Stokes S_1,S_2,S_3	input	input	input	input	calc.	input	input	input	file	input	input

Table 1 **Main parameters of the *RAY*-sources**
(*hard*: a hard edge; *soft*: a gaussian distribution of the respective variable within a 6σ-width is simulated; *calc:* calculated according to a theoretical model (e.g. Schwinger theory)*; n*: number of Wiggler periods, *L* length of undulator, λ_u: period length.)

The source coordinate system for the case of bending magnet synchrotron radiation is given in Fig. 3. The storage ring is located in the *x-z* plane, for clockwise revolution of the electrons the x-axis is pointing away from the center, while for counter-clockwise revolution the x-axis is pointing inside the storage ring center. This is important to be noticed especially for optical systems with large horizontal divergence (e.g. IRbeamlines), when the source cross section is getting asymmetrical because of the depth of field effect (see figure 3).

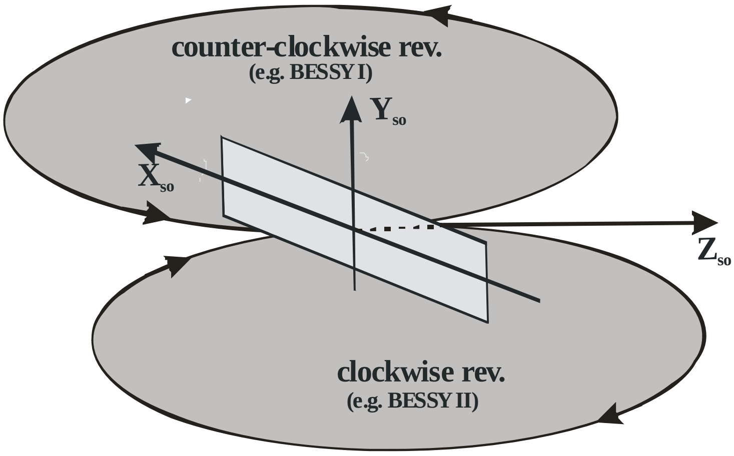

Figure 3 Coordinate system for storage ring-bending magnet sources (DI_pole)

Examples of the intensity distribution (footprints) of various sources are given in the figures 4 and 5.

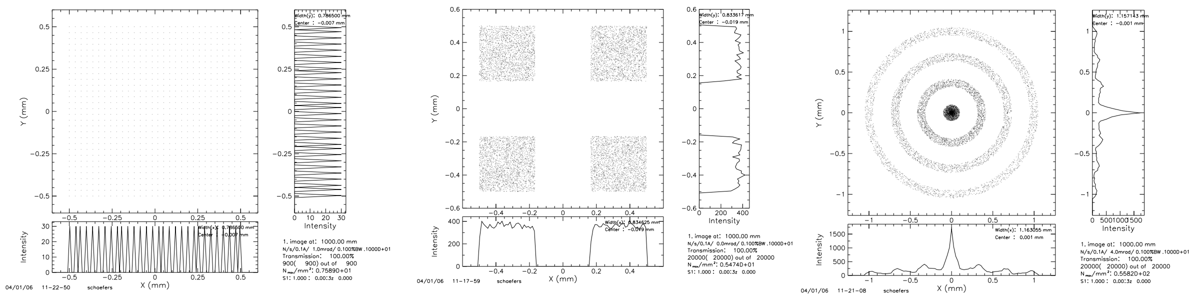

Figure 4 Spot pattern of various Source types
MA_trix PI_xel CI_rcle

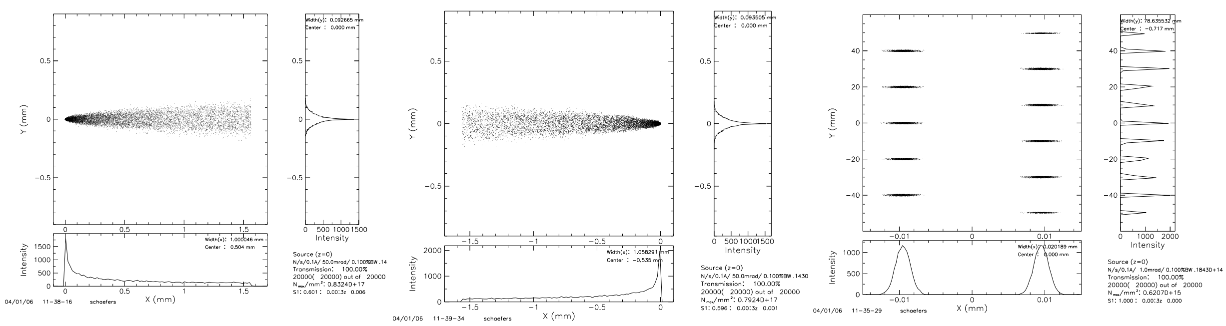

Figure 5 Spot pattern of synchrotron radiation sources
DI_pole, clockwise rev. DI_pole, counter-clockw. rev. WI_ggler, seen from top (x-z plane)

3.3 Geometry

The definition of the coordinate system used in *RAY* is shown in Figs. 6 and 7. The coordinate system is transformed along the optical path from the source to the optical elements and then to the image planes. Its origin lies in the center of the source, (with the x-axis in general (e.g. SR) being horizontal) the optical elements or the image planes, respectively. The *z*-axis points into the direction of the central ray, the *x*-axis is perpendicular to the plane of reflection, i.e. horizontal in the case of a vertically deviating optical setup (azimuthal angle 0° or 180°), and vertical for horizontal mounts (azimuthal angles 90° (to the right) and 270° (to the left), respectively). The *y*-axis is *always* the normal in the center of the optical element. The plane of reflection or dispersion is, thus, *always* the *y*-*z* plane. The surface of the optical elements is *always* the *x*-*z*-plane, regardless of the azimuthal angle χ. After the optical element the coordinate system for the outgoing ray is rotated back by -χ, i.e. it has the same orientation as before the optical element.

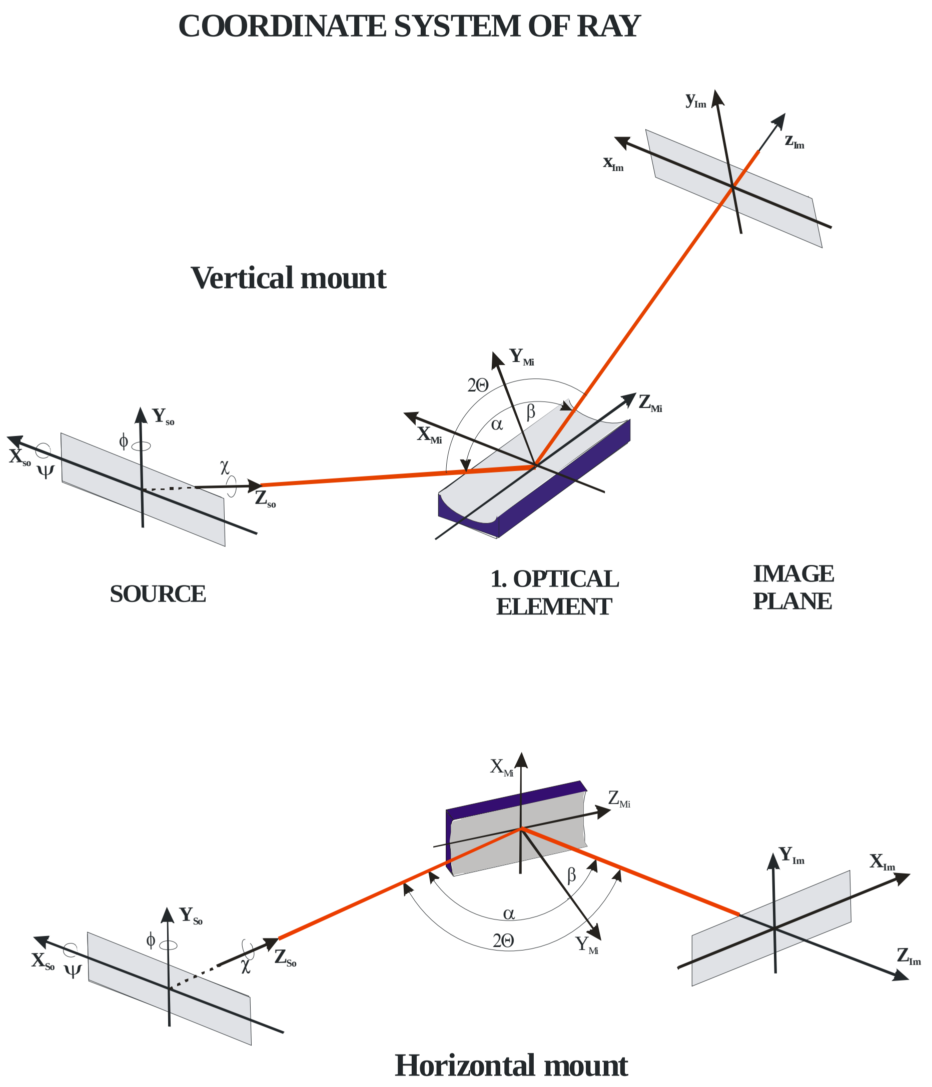

Figure 6 Coordinate system (right handed screw) and angles used in RAY. Top: vertical deviation (upwards (downwards)) mount (azimuthal angle χ=0° (180°)), Bottom: horizontal deviation (to the right (left)) (azimuthal angle χ=90° (270°)). The optical element is always in the X_M-Z_M-plane.

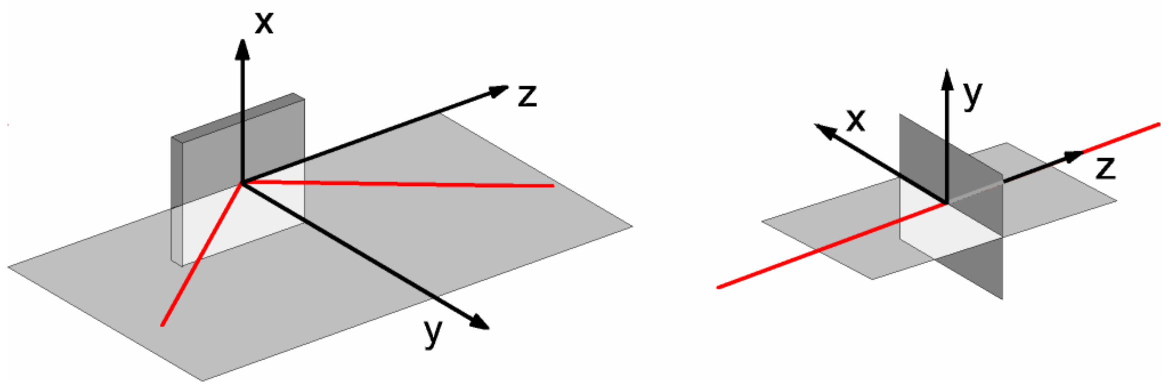

Figure 7: Coordinate systems used in RAY. For optical elements (left) the coordinate system is fixed to the optical surface (X-Z plane). Transmission elements, screens and image planes (right) are in the X-Y plane, the x-axis is in the horizontal plane.

The geometric calculations proceed in the following way:

1) Statistical creation of a ray within a given source volume and emission cone and within the 'correct' statistics (see 3.1). The ray is determined by its source coordinates (x_s,y_s,z_s) and its direction cosines (l_s,m_s,n_s), determined by the horizontal and vertical emission angles φ and ψ (see figure 8):

$$\vec{\alpha}_S = \begin{pmatrix} l_S \\ m_S \\ n_S \end{pmatrix} = \begin{pmatrix} \sin\varphi\cos\psi \\ \sin\psi \\ \cos\varphi\cos\psi \end{pmatrix} \tag{3}$$

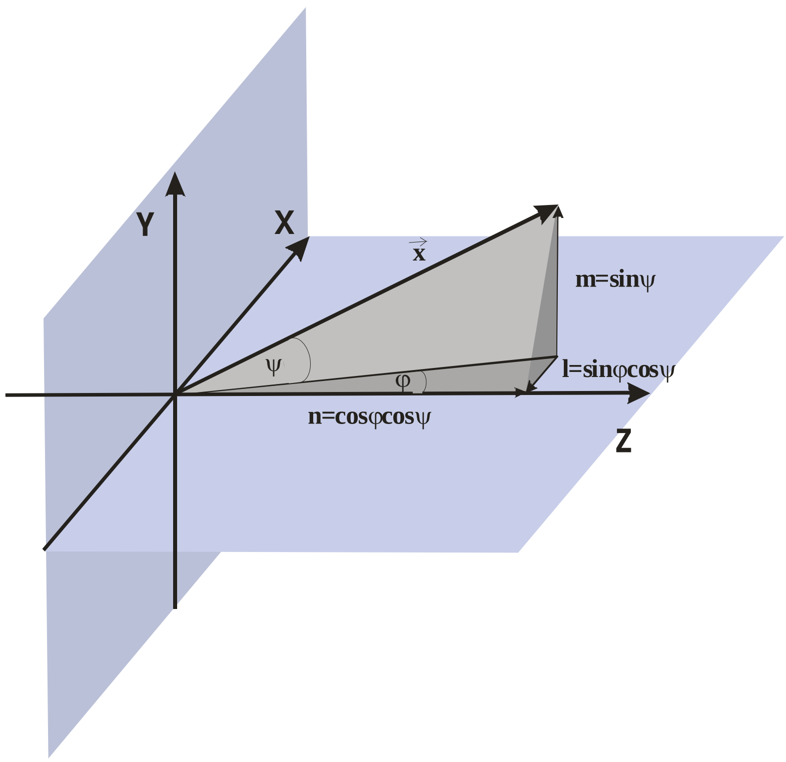

Figure 7

Source coordinate system: Definition of angles and direction cosini in RAY

The vector equation of the ray is then

$$\vec{x} = \vec{x}_S + t\vec{\alpha}_S \tag{4}$$

or, in coordinates:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x_s \\ y_s \\ z_s \end{pmatrix} + t \begin{pmatrix} l_S \\ m_S \\ n_S \end{pmatrix} \tag{5}$$

or

$$\frac{x - x_s}{l_S} = \frac{y - y_s}{m_S} = \frac{z - z_s}{n_S} \tag{6}$$

2) Transformation of the source-coordinate system to a new coordinate system with the origin in the center of the 1st optical element (hit by the central ray), and the z-axis parallel to a symmetry-axis of the optical element (for a simplified equation). The coordinate system is translated by the '*distance from the source*' to the optical element, z_q, rotated around z by the azimuthal angle, χ, and around the new $\tilde{x}$ -axis by the grazing incidence angle θ. The transformation to the new-coordinate system is performed by the following matrix-operations:

$$\vec{x}_{S'} = D_{\tilde{x}}(\theta) D_z(\chi) T_z(z_q) \cdot \vec{x}_S \tag{7}$$

z_q	distance source to 1st optical element or n-th to (n+1)st element
θ	rotation angle around x (y-z plane)
χ	azimuthal rotation around z (x-y plane) counted clockwise

which corresponds to:

$$\begin{pmatrix} x_{S'} \\ y_{S'} \\ z_{S'} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix} \circ \begin{pmatrix} \cos\chi & -\sin\chi & 0 \\ \sin\chi & \cos\chi & 0 \\ 0 & 0 & 1 \end{pmatrix} \circ \left(\begin{pmatrix} x_S \\ y_S \\ z_S \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ z_q \end{pmatrix} \right) \tag{8}$$

or, finally:

$$\begin{pmatrix} x_{S'} \\ y_{S'} \\ z_{S'} \end{pmatrix} = \begin{pmatrix} x\cos\chi - y\sin\chi \\ x\sin\chi\cos\theta + y\cos\chi\cos\theta - (z - z_q)\sin\theta \\ x\sin\chi\sin\theta + y\cos\chi\sin\theta + (z - z_q)\cos\theta \end{pmatrix} \tag{9}$$

The direction cosines are transformed correspondingly:

$$\vec{\alpha}_{S'} = D_{\tilde{x}}(\theta) D_z(\chi) \cdot \vec{\alpha}_S \tag{10}$$

and finally:

$$\begin{pmatrix} l_{S'} \\ m_{S'} \\ n_{S'} \end{pmatrix} = \begin{pmatrix} l\cos\chi - m\sin\chi \\ l\sin\chi\cos\theta + m\cos\chi\cos\theta \\ l\sin\chi\sin\theta + m\cos\chi\sin\theta \end{pmatrix} \tag{11}$$

In the new coordinate system the ray is described by:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}(t) = \begin{pmatrix} x_{S'} \\ y_{S'} \\ z_{S'} \end{pmatrix} + t \begin{pmatrix} l_{S'} \\ m_{S'} \\ n_{S'} \end{pmatrix} \tag{12}$$

3) A 6-dimensional misalignment of an optical element can be taken into account: three translations of the coordinate system by δx, δy *and* δz and three rotations by the misorientation angles $\delta\chi$ (*x*-*y* plane), and $\delta\varphi$ (*x*-*z* plane) and $\delta\psi$ (*y*-*z* plane). Since the rotations are not commutative, the coordinate system is first rotated by these angles in the given order and then translated. For the outgoing ray to be described in the non-misaligned system, the coordinate system is backtransformed (in reverse order). Thus the optical axis remains unaffected by the misalignment.

4) In this coordinate system the optical element is described by the general equation for 2nd-order surfaces:

$$\begin{aligned} &F(x,y,z) = \\ &= a_{11}x^2 + a_{22}y^2 + a_{33}z^2 + \\ &+2a_{12}xy + 2a_{13}xz + 2a_{23}yz + \\ &+2a_{14}x + 2a_{24}y + 2a_{34}z + a_{44} = 0 \end{aligned} \tag{13}$$

This description refers to a right-handed coordinate system attached to the center of the mirror with its surface in x-z plane, y-axis points to the normal). This coordinate system is used for the optical elements PL_ane, CO_ne, CY_linder and SP_here.

The individual surfaces are are described by the following equations:

a) Plane	$y = 0$
b) Cylinder (in z.dir)	$x^2 + y^2 = 0$
b) Cylinder (in x-dir.)	$y^2 + z^2 = 0$
c) Cone	
c) Sphere	$x^2 + (y-R)^2 + z^2 - R^2 = 0$
d) Ellipsoid	$x^2/C^2 + (y-y_o)^2/B^2 + (z-z_o)^2/A^2 - 1 = 0$
e) Paraboloid	$x^2/C^2 + (y-y_o)^2/B^2 - 2P(z-z_o) = 0$ (14)

Note that for the elements EL_lipsoid and PA_raboloid a coordinate system is used which again is attached to the center of the mirror, (with x-axis on the surface) but the z-axis is parallel to the symmetry axis of this element for an easier description in terms of the a_{ij} parameters (see figures 9 and 10). The a_{ij}-values of the table 2 are given for this system. Thus, the rotation angle of the coordinate system from source to element is here $\theta+\alpha$ (EL) and 2θ (PA), respectively, θ being the grazing incidence angle and α the tangent angle on the ellipse.

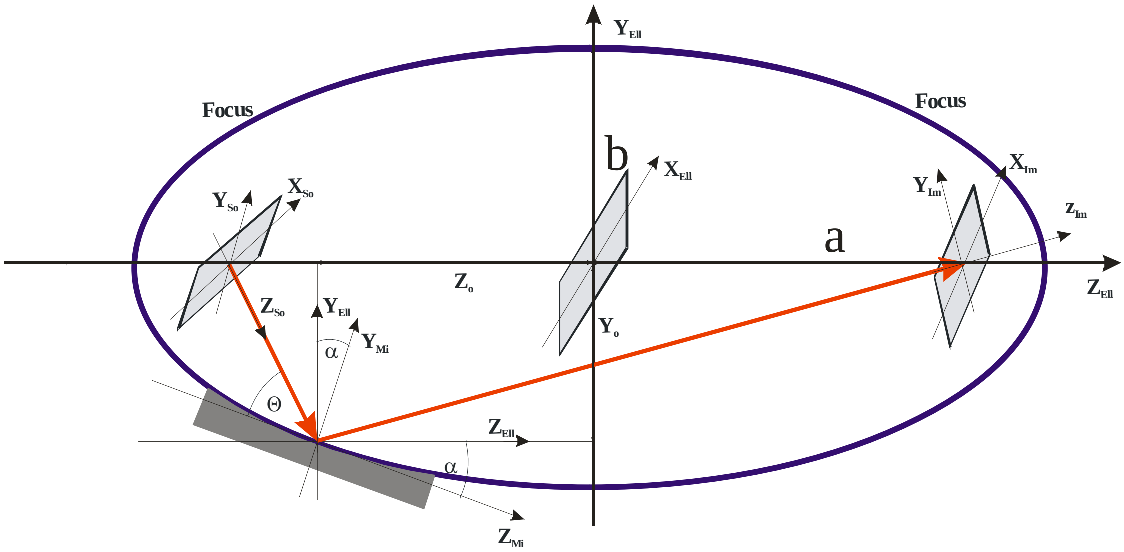

Figure 9 Ellipsoidal mirror: Definitions and coordinate systems

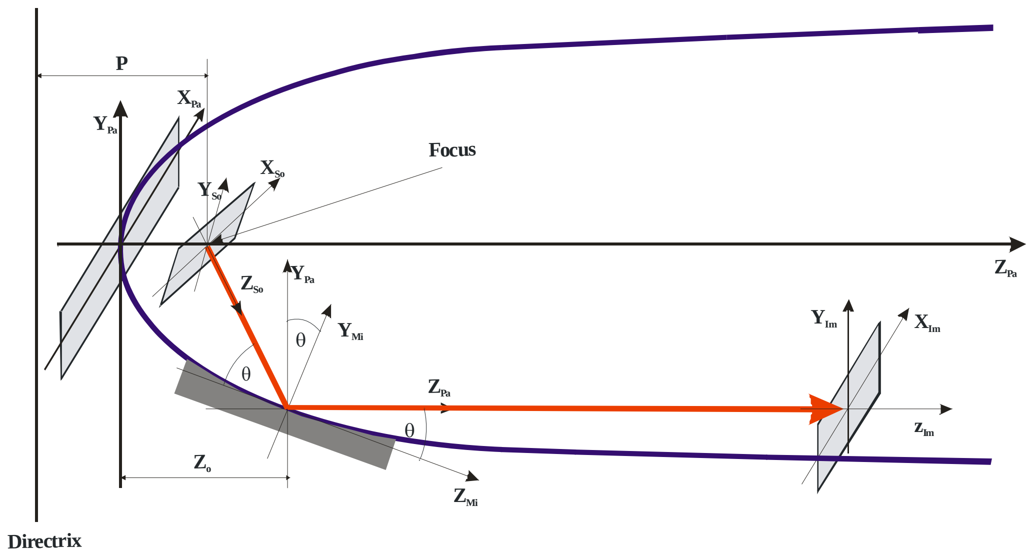

Figure 10 Paraboloid mirror: Definitions and coordinate systems

For the higher order surfaces the surface is described by the following equations:

a) Toroid:

$$F(x,y,z)=\left((R-\rho)+sign(\rho)\sqrt{\rho^2-x^2}\right)^2-(y-R)^2-z^2=0 \qquad (15)$$

sign=+/-1 for concave/ convex curvature.

The surface normal is calculated according to (see section 3.6):

$$F_x = \frac{-2x\,sign(\rho)}{\sqrt{\rho^2 - x^2}}\left((R-\rho) + sign(\rho)\sqrt{\rho^2 - x^2}\right)^2 \tag{16}$$

$$F_y = -2(y - R) \tag{17}$$

$$F_z = -2z \tag{18}$$

b) Elliptical paraboloid:

$$F(x,y,z) = \frac{2fx^2}{2f - \frac{z+z_0}{\cos 2\theta}} - 2p(z+z_0) - p^2 = 0 \tag{19}$$

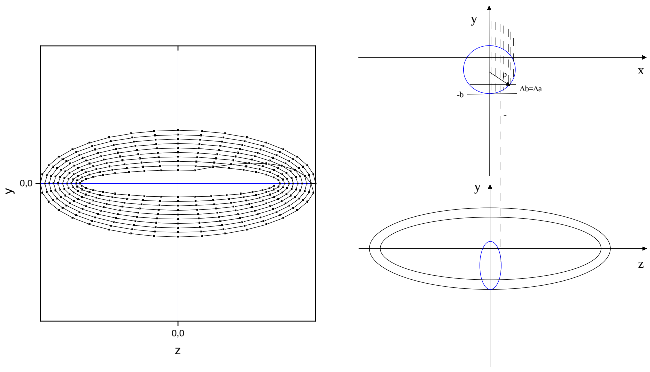

Figure 11 construction of an elliptical torus

c) Elliptical toroid:

A small radius ρ in the (x,y)-plane is traced along the ellipse in the (y,z)-plane. Each point of the circle is origin of a new and smaller ellipse in the (y,z)-plane with the half-axis parameters a-Δb and b-Δa (see Fig. 11). The surface described in the coordinate system of the ellipse is given by:

$$F(x,y,z) = z^2(b-\rho+\sqrt{\rho^2-x^2})^2 + y^2(a-\rho+\sqrt{\rho^2-x^2})^2 - $$
$$-(a-\rho+\sqrt{\rho^2-x^2})^2(b-\rho+\sqrt{\rho^2-x^2})^2 = 0 \tag{20}$$

with the surface normal given by:

$$F_x = -2z^2x\frac{(b-\rho+\sqrt{\rho^2-x})}{\sqrt{\rho^2-x^2}} - 2y^2x\frac{(a-\rho+\sqrt{\rho^2-x^2})}{\sqrt{\rho^2-x^2}}^2 +$$
$$+2x\frac{(a-\rho+\sqrt{\rho^2-x})(b-\rho+\sqrt{\rho^2-x^2})}{\sqrt{\rho^2-x^2}}((b-\rho+\sqrt{\rho^2-x^2})+(a-\rho+\sqrt{\rho^2-x^2})) \tag{21}$$

$$F_y = -2y(a-\rho+\sqrt{\rho^2-x})^2 \tag{22}$$

$$F_z = -2z(b-\rho+\sqrt{\rho^2-x})^2 \tag{23}$$

The definition of variables corresponds to the paraboloid (see table 2). The intersection point is determined by an iteration procedure.

For the different mirror types the coefficients a_{ij} have the following values:

Name	**PM**	**CY**	**CO**	**SP**	**EL**	**PA**
$\mathbf{a_{11}}$	*0*	*1/0*	$1\text{-}c_m$	*1*	B^2/C^2	P^2/C^2
$\mathbf{a_{22}}$	*0*	*1*	$1\text{-}2c_m$	*1*	*1*	*1*
$\mathbf{a_{33}}$	*0*	*0/1*	*0*	*1*	B^2/A^2	*0*
$\mathbf{a_{12}}$	*0*	*0*	*0*	*0*	*0*	*0*
$\mathbf{a_{13}}$	*0*	*0*	*0*	*0*	*0*	*0*
$\mathbf{a_{23}}$	*0*	*0*	$\sqrt{c_m - c_m{}^2}$	*0*	*0*	*0*
$\mathbf{a_{14}}$	*0*	*0*	*0*		*0*	*0*
$\mathbf{a_{24}}$	*-1*	$\rho\cdot sign$	$-a_{23}\frac{R}{\sqrt{c_m}} - \frac{z_m}{2}$	$R\cdot sign$	$-y_0$	$-y_0$
$\mathbf{a_{34}}$	*0*		*0*	*0*	$z_0\cdot B^2/A^2$	$-P$
$\mathbf{a_{44}}$	*0*	*0*	*0*	*0*	$y_0^2+z_0^2\cdot B^2/A^2-B^2$	$y_0^2-2Pz_0-P^2$
sign **(concave/convex)**	*0*	*1/-1*	*1/-1*	*1/-1*	*1*	*1*
$\mathbf{F_x}$ $-(a_{11}x+a_{12}y+a_{13}z+a_{14})$	*0*	$-x\ /\ 0$		$-x$	$-a_{11}x$	$-a_{11}x$
$\mathbf{F_y}$ $-(a_{22}y\cdot sign+a_{12}x$ $a_{23}z+a_{24})$	*1*	$\rho\cdot sign$		$R\cdot sign$	y_0-y	y_0-y
$\mathbf{F_z}$ $-(a_{33}z+a_{13}x+a_{23}y+a_{34})$	*0*	$0\ /\ -z$		$-z$	$-(z_0+z)\cdot(B/A)^2$	P
					$z_0=A^2/B^2y_0\tan(\alpha)$	$z_0=f\cdot\cos(\alpha,\beta)\cdot sig$
					$y_0=r_a\sin(\theta-\alpha)$	$y_0= f\cdot\sin(2\alpha,\beta)$
					$\tan(\alpha)=\tan(\theta)\cdot$ $\cdot(r_a-r_b)/(r_a+r_b)$	$P=2f\sin^2(\theta)sig$
		ρ: *radius*	R, ρ: *radii*	R: *radius*		*f: mirror - source /focus - dist.*
			z_m: *mirror length* $c_m = (\frac{(r-\rho)}{z_m})^2$		*A, B, C half axes in z,y,x-dir.* r_a, r_b: *mirror to focus 1,2* θ: *grazing angle of central ray* α=*tangent angle*	*C: halfpar. in x* *sig =+/-1* *f. collimation/ focussing* θ: *grazing angle of central ray* $\alpha,\beta=2\theta$, *0 (coll)* $\alpha,\beta=0$, 2θ *(foc.)*
					Plane Ell.: C=infty. *Rotational Ell.: B=C<>A* *Ellipsoid: A≠B≠C* *Sphere: A=B=C*	*Plane P.: C=infty.* *Rotational P.: C=P* *Elliptical P.: C≠P*

Table 2 **Parameters of the optical elements in *RAY***

5) Calculation of the intersection point (x_M,y_M,z_M) of the ray with the optical element by solving the quadratic equation in t generated by inserting equation (12) into (13)
6) Determination of the surface normal for this point $\vec{n} = n(x_M,y_M,z_M)$ by calculating the partial derivative of $F(x_M,y_M,z_M)$:

$$\vec{f} = \nabla F \tag{24}$$

with the components: $$f_x = \frac{\partial F}{\partial x} \qquad f_y = -\frac{\partial F}{\partial y} \qquad f_z = \frac{\partial F}{\partial z} \tag{25}$$

The surface normal is then given by the unit vector:

$$\vec{n} = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} = \frac{1}{\sqrt{f_x{}^2 + f_y{}^2 + f_z{}^2}} \begin{pmatrix} f_x \\ f_y \\ f_z \end{pmatrix} \tag{26}$$

7) Figure and finish errors, thermal distortion:
the surface normal is modified incrementally by rotating the normal vector in the *y*-*z* (meridional plane) and in the *x*-*y* plane (sagittal). The determination of the rotation angles depends on the type of error to be included:

a) Slope errors, microroughness: the rotation angles are chosen statistically (according to the procedure described in 3.1) within a 6σ-width of the input value for the slope error.
b) Thermal bumps: a gaussian height profile in *x*- and *z*-direction with a given amplitude and σ-width can be put on the mirror center.
c) Cylindrical bending: a cylindrical profile in *z*-direction (dispersion direction) with a given amplitude can be superimposed onto the mirror surface.
d) Measured surface profiles, e.g. by a profilometer.
e) Surface profiles calculated separately e.g. by a finite element analysis program.

In cases b)-e) the modified mirror surface is stored in a *100*x*100* matrix representing the amplitudes (*y*-coordinates). For cases b) and c) this matrix is calculated within *RAY*, for the cases d) and e) ASCII-data-files can be read according to the file structure of the *M400*-surface profilometer data /27/ and the *ANSYS*-Finite Element analysis data /24/ (see appendix A4).

8) Calculation of the direction cosines of the reflected/transmitted/refracted ray $(\vec{\alpha}_2)$ =(l_2,m_2,n_2) from the incident ray $(\vec{\alpha}_1)$ =(l_1,m_1,n_1) and the surface normal $\vec{n}$ *:*

a) For reflection mirrors and crystals the entrance angle α is equal to the exit angle β. In vector notation this means that the cross product is

$$\vec{n} \, \mathrm{x} \, (\vec{\alpha}_2 - \vec{\alpha}_1) = 0 \tag{27}$$

since the two vectors are parallel. For the direction cosines of the reflected ray the result is given by

$$\vec{\alpha}_2 = \vec{\alpha}_1 - 2 \cdot (\vec{n} \circ \vec{\alpha}_1) \circ \vec{n} \tag{28}$$

or, for the coordinates

$$l_2 = l_1 - 2n_x \frac{\ln_x + mn_y + nn_z}{n_x{}^2 + n_y{}^2 + n_z{}^2} \tag{29}$$

and, correspondingly for m_2 and n_2.

b) For gratings by applying the grating equation

$$k\lambda = d(\sin\alpha + \sin\beta). \tag{30}$$

1. The grating is rotated by $\delta\chi = atan(n_x/n_y)$ around the *z-axis* and by $\delta\psi = asin(n_z)$ around the *x*-axis, so that the intersection point is plane (surface normal parallel to the y-axis). The grating lines are parallel to the *x*-direction.

2. Then the direction cosines of the diffracted beam are determined by

$$\begin{pmatrix} l_2 \\ m_2 \\ n_2 \end{pmatrix} = \begin{pmatrix} l_1 \\ \sqrt{m_1^{\ 2} + n_1^{\ 2} - (n_1 - a_1)^2} \\ n_1 - a_1 \end{pmatrix} \tag{31}$$

$a_1 = k \dfrac{\lambda}{d} \cos\delta\psi$,   *k*: diffraction order, λ: wavelength, *d*: grating constant

3. The grating is rotated back by to the original position by $-\delta\psi$ *and* $-\delta\chi$.

For varied line-spacing (VLS-)gratings the actual line density *n =1/d (l/mm)* as a function of the position is determined by

$$n = n_0 \cdot \left(1 + 2b_2 z + 3b_3 z^2 + 4b_4 z^3 + 2b_5 x + b_6 z + b_6 xz + 4b_7 x^3\right). \tag{32}$$

c) For transmitting optics the direction of the ray is unchanged.

9) Rotation of the coordinate system by the reflection angle $-\theta$ and the azimuthal angle $-\chi$, such that the *z*-axis follows once again the direction of the reflected central ray as it was for the incident ray. The old values of the source/mirror points and direction cosines are replaced by these new ones, so that new optical elements can be put one after the other (see 2).

10) If the ray has traversed the entire optical system the intersection points (x_I, y_I) with up to 3 image planes at the distances $z_{I_{1,2,3}}$ are determined according to

$$\begin{pmatrix} x_I \\ y_I \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix} + \frac{1}{n}\begin{pmatrix} l \\ m \end{pmatrix}(z_{I_{1,2,3}} - z)\,. \tag{33}$$

11) For imaging systems, if the focus position is to be determined and displayed, the *x*- and *y*-coordinates of that ray which has the largest coordinates are stored along the light beam for a graphic display of the cross section of the beam.

12) Data evaluation and storage. The *x, z*-coordinates (*x, y* for source, slits, foils, zoneplates and image planes) and the angles *l, n (l, m,* respectively), are fed into two-dimensional *100*x*100* integer-matrices. These matrices are multichannel arrays, one for each element, whose dimensions have been fixed in a ‘test-raytrace’ run. They represent the illuminated surface of the element in *x-z* projection. The corresponding surface element which has been hit by a ray is increased by 1, so that later the intensity pattern on the element can be displayed.
Additionally, the *x*- and *z*-coordinates (*y*, respectively, s.a.) of the first 10.000 rays are stored in a real *10.000x2* matrix for display of the footprint patterns on the optical elements or for point diagrams at the image planes.

13) Start with a new ray according to 3.3.1 (above).

3.4 Optics

Not only the geometrical path of the rays is followed throughout an optical setup, but also the intensity and polarization properties of each ray are traced. Thus, it is easily possible to simulate depolarization effects throughout the optical path, or optimize an optical setup for use as a polarization monitor. For this, each ray is treated individually with a defined energy and polarization, without any interference with other rays. Thus, collective effects like interference and diffraction are explicitely NOT taken into account.

RAY employs the Stokes formalism for this purpose. The Stokes vector $\vec{S}=(S_0,S_1,S_2,S_3)$ describing the polarization (S_1,S_2: linear, S_3: circular polarization) for each ray is either given as free input parameter or, for dipole sources, it is calculated according to the Schwinger theory. S_0, the start intensity of the ray from the source $(S_0 = \sqrt{S_1^{\,2} + S_2^{\,2} + S_3^{\,2}})$ is set to 1 for the artificial sources. It is set to a realistic photon flux value for the sources like Dipole, Wiggler or the Undulator File sources.

The Stokes vector is defined by the following equations:

$$
\begin{aligned}
S_0 &= \left[\left(E^o{}_p\right)^2 + \left(E^o{}_s\right)^2\right]/2 & &= 1 \\
S_1 &= \left[\left(E^o{}_p\right)^2 - \left(E^o{}_s\right)^2\right]/2 & &= P_l \cos(2\delta) \\
S_2 &= E^o{}_p E^o{}_s \cos\left(\phi_p - \phi_s\right) & &= P_l \sin(2\delta) \\
S_3 &= -E^o{}_p E^o{}_s \sin\left(\phi_p - \phi_s\right) & &= P_c
\end{aligned}
\qquad (34)
$$

with the two components of the electric field vector defined as

$$E_{p,s}(z,t) = E^o_{p,s} \exp\left[i\left(\omega t - kz + \phi_{p,s}\right)\right]. \qquad (35)$$

and P_l, P_c are the degree of linear and circular polarisation, respectively. δ is the azimuthal angle of the major axis of the polarisation ellipse. Note that

$$P_l, = P \cos(2\varepsilon) \qquad (36)$$
$$P_c, = P \sin(2\varepsilon) \qquad (37)$$

With P being the degree of total polarisation, and ε the ellipticity of the polariation ellipse ($\tan\varepsilon = R_p/R_s$).

Since the SR is linearly polarised within the electron orbital plane $(I_{perp}=0)$, the plane of linear polarisation is thus coupled to the x-axis (i.e. horizontal). Thus the Stokes-Vector for SR is in our geometry defined as (see chapter 3.4):

$$P_{lin} = S_1 = (I_{perp}-I_{par})/(I_{perp}+I_{par}) = (I_y-I_x)/(I_y+I_x) = -$$
(38)

$S_1=+1$ would correspond to a vertical polarisation plane.

For the definition of the circular polarisation the nomenclature of Westerfeld et al./28/ and Klein/Furtak /29/ has been used. This is summarised in table 3:

Phase ϕ_{p-s}	***90º, -270º*** ***π/2, -3π/2***	***-90º, 270º*** ***-π/2, 3π/2***
Rotation sense (in time)	clockwise	counter-clockwise
Rotation sense (in space)	counter-clockwise	clockwise
Polarisation (optical def.)	R(ight) CP	L(eft) CP
Helicity (atomic def.)	negative (σ-)	positive (σ+)
Stokes vector	negative	positive

Table 3 Definition of circular polarisation acc. to /28/ and /29/

So, for the case of synchrotrons and storage rings, the radiation, which is emitted off-plane, upwards, has negative helicity, right-handed CP (S_3=-*1*), when the electrons are travelling clockwise, as seen from the top.

The modification of the Stokes vector throughout the beamline by interaction of the light with the optical surface is described by the following steps /see e.g. 28/:

1) Give each ray a starting value for the Stokes parameter within the source S_{ini}

2) Calculate the intensity losses at the first optical element for *s*- and *p*-polarization geometry, and the relative phase $\Delta=\delta_s-\delta_p$, according to the physical process involved (see table 4):

Mirrors	**Gratings**	**Foils**	**Slits**	**Zoneplates**	**Crystals**
Fresnel equations	diffraction theory	Fresnel equations	-	-	dynamic theory
Reflectance	Efficiency	Transmission	Transmission	Transmission	Reflectance
R_s, R_p, Δ_{sp}	E_s, E_p, Δ_{sp}	T_s, T_p, Δ_{sp}	T_s,T_p=1,Δ_{sp}=0	T_s,T_p=1,Δ_{sp}=0	R_s, R_p, Δ_{sp}

Table 4 **Physical interaction for the different optical components**

3) Transform the incident Stokes vector, $\vec{S}_{ini}$, into the coordinate system of the optical element $\vec{S}_M$ by rotation around the azimuthal angle χ (*R*-matrix)

$$\vec{S}_M = R_{\tilde{y}}(\chi)\cdot\vec{S}_{ini} \tag{39}$$

$$\vec{S}_M = \begin{pmatrix} S_{0M} \\ S_{1M} \\ S_{2M} \\ S_{3M} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\chi & \sin 2\chi & 0 \\ 0 & -\sin 2\chi & \cos 2\chi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \bullet \begin{pmatrix} S_{0ini} \\ S_{1ini} \\ S_{2ini} \\ S_{3ini} \end{pmatrix}. \tag{40}$$

4) Calculate the Stokes vector after the optical element $\vec{S}_{final}$ by applying the Müller matrix, *M,* onto $\vec{S}_M$

$$\vec{S}_{final} = M \cdot \vec{S}_M \tag{41}$$

$$\begin{pmatrix} S_{0\,final} \\ S_{1\,final} \\ S_{2\,final} \\ S_{3\,final} \end{pmatrix} = \begin{pmatrix} \frac{R_s + R_p}{2} & \frac{R_p - R_s}{2} & 0 & 0 \\ \frac{R_p - R_s}{2} & \frac{R_s + R_p}{2} & 0 & 0 \\ 0 & 0 & R_s R_p \cos\Delta & R_s R_p \sin\Delta \\ 0 & 0 & -R_s R_p \sin\Delta & R_s R_p \cos\Delta \end{pmatrix} \circ \begin{pmatrix} S_{0M} \\ S_{1M} \\ S_{2M} \\ S_{3M} \end{pmatrix}. \tag{42}$$

5) Accept this ray only when its intensity ($S_{0,final}$) is within the 'correct' statistic, i.e. when

$$(S_{0,final}/S_{0,ini} - ran(z)) > 0. \tag{43}$$

6) Rotate the Stokes vector $\vec{S}_{final}$ back by $-\chi$ and take this as incident Stokes vector for the next optical element

$$\vec{S}'_{ini} = R_{\tilde{y}}(-\chi) \cdot \vec{S}_{final}\,. \tag{44}$$

7) Store the Stokes vector for this optical element, go to the next one (2) or start with the next ray within the source (1).

4. Getting started

The program runs on either Open VMS/VAX or Open VMS/Alpha and has been tested up to VMS-version 6.2. The graphics output can be displayed on any X11-display, it can be sent to a Postscript-printer or saved in a PS or EPS file. It is possible to write the resulting data to ASCII files for input to other programs. The parameters for the calculation can be stored in a parameter file which is a very efficient way if complex calculations have to be repeated later with minor modifications.

RAY can be called from anyone of the BESSY-I or BESSY-II Open VMS-cluster or cluster-connected PC-terminals. You just have to be logged in on your user-account at the BESSY-DEC-computer-system.

4.1 Call on your BESSY-Account

1) The installation of *RAY* on your BESSY-computer account is done by calling the comand-procedure

   @PRG:RAY_SETUP

2) If you work outside BESSY, you must specify the graphic output of the program to your terminal before starting by

   SET DISPLAY/CREATE/TRANSPORT=TCPIP/NODE=<your IP-Hostname>

   For frequent users of *RAY* it is preferable to include these two lines to the *LOGIN.COM*-file.

3) *RAY* is then started by

   RUN PRG:RAY or simply by ***RAY***

4.2 Your personal installation

1) Before starting *RAY* you may define your preferred printers as the logicals *RAY_PRINTER_PS1* and *-2* by

   DEFINE/NOLOG RAY_PRINTER_PS1 YOURPRINTER1
and ***DEFINE/NOLOG RAY_PRINTER_PS2 YOURPRINTER2,*** respectively.

2) To save disk space during printing, the logical *SYS$SCRATCH* can be defined as

   DEFINE/NOLOG SYS$SCRATCH BESSY$SCRATCHDISK:[YOURNAME]

4.3 PC-Windows Version of RAY

The PC-Windows version has been tested up to WINDOWS XP. It is running in a DOS-box and it is a 1:1 copy of the VAX/ALPHA version with no change in the interactive input menue. At BESSY it is available via network in the open diskdrive ‘Public auf BESSY’ under the adress

P:\RayReflec\RAY.exe

The executable version including all optical constants data-files within the necessary directory structure is available at request as ZIP-file for out-of-BESSY installation.

5. Summary of the features of *RAY*

Raytracing

- **imaging/focusing properties of optical systems**
  - **create rays within a source volume**
  - **trace them through optical elements**
  - **display geometric distribution of rays at focus**
- **design tool for SR beamlines: ((V)UV, (soft) x ray**
  - **dipole radiation (bending magnets)**
  - **3rd generation Wiggler/Undulator beamlines**
  - **including helical undulators**
- **also for general optical applications**
- **predict performance under realistic (non-ideal) conditions**
- **specify requirements before order of optical elements**
- **indispensible tool for modern beamline design**
- **RAY,REFLEC - userfriendly**
  - easy accessible
  - self explaining menue
  - easy to learn
  - no file handling
  - every day use
- **FORTRAN source code written for**
  - **Open VMS (V. 7.1) under VAX/Alpha**
  - **PC-Windows 95, 98, NT, 2000**
- **on-line graphic on monitor**
  - **hardcopy on LPT1, 2**
  - **ASCII-, PS-, EPS-files**

- **A RAY described by**
  - **geometric coordinates**
  - **emission angle**
  - **energy**
  - **polarisation**
  - **pathlength**

- **SOURCES**
  - **Synchr.Rad.: Dipole - WLS -Wiggler - (helical, double) Undulator**
  - **Point - Pixel pattern - Circle - ASCII-file**
  - **realistic simulation of source volume and emission characteristic**
  - **for SR sources: - polarisation included**
    - electron beam emittance effects
    - detuning effects (orbit change, misalignment)
  - **Monte-Carlo random feature for intensity simulation**

- **OPTICAL ELEMENTS**
  - **transmitting - Slits, Foils**
  - **reflecting - Mirrors, multilayers**
  - **dispersing - Gratings, Zoneplates**
  - **diffracting - Crystals**
  - **Optical constants data tables from near-UV to hard x-rays**
    (Palik, Henke, Cromer, Crystal structure factors)
  - **Special mounts: - SX700 plane grating PGM**
    - spherical grating SGM
    - Varied Line Spacing-(VLS-) gratings
    - laterally graded crystals, multilayers
  - **Surface figures - plane, cylinder, sphere, toroid**
    - conus, ellipse, parabloid
  - **Miscellaneous: - misalignment of source / optics**
    - slope errors, surface roughness
    - thermal deformation
    - surface profiles

- **IMAGE PLANES: screens after last optical element**

- **DISPLAY features:**
  - **focus position**
  - **footprint of light on the optics**
  - **spatial distribution (spot pattern)**
  - **intensity profiles**
  - **angular distribution**
  - **energy resolution**
  - **absolute transmission**

- **flux, flux density, (de-)polarisation**

- **Program Input**
  - -- Interactive, batch or by parameter-file
  - -- Specification of source, beamline (up to 10 optical elements) and image planes

- **Program output**
  - -- Graphical display of results on VT100, DEC-Term, X11-display, PC-terminals
  - -- ASCII-datafiles
  - -- Hardcopy, PS-Files, EPS-Files
  - -- Parameter File for all input data

- **Display Features**
  - -- Point diagrams (spot pattern) at source, optical elements (footprints) and image planes
  - -- Horizontal and vertical intensity profiles
  - -- Focus position
  - -- Horizontal and vertical angular distribution of rays
  - -- Energy distribution and resolution

- **Hardware**
  - -- DEC-VAX or ALPHA with open VMS or PC-WINDOWS
  - -- At BESSY the *RAY.EXE* versions are installed on the general user-accounts PRG:
  - -- Program-call from any account at any VAX, Alpha or network-PC-terminal by
    RUN PRG:RAY
  - -- WINDOWS: Public diskdrive at BESSY ***P:\RayReflec\RAY.exe***

- **Software installation**
  - -- BESSY-Graphic-library *PLT96*
  - -- Logicals: *RAY_OPTCON, SYS$SCRATCH*
  - -- *RAY_SETUP.COM*-Commandfile for individual installation of Printerqueues *RAY_PRINTER_1* and *2*, resp.

- **Source-Program-Packages**
  - -- *RAY.FOR*
  - -- *ALPHA_ROUTINES.FOR* or *PC_ROUTINES.FOR*
  - -- *CRYSUB.FOR*
  - -- *OEINPUT.FOR*
  - -- *OPTCON.FOR*
  - -- *OPTICS.FOR*
  - -- *RAYLIB.FOR*
  - -- *SOURCE.FOR*
  - -- *PLT96.LIB or HIGS library*

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26. OPTIMO - software code to optimize VUV/X-ray optical elements, developed by F. Eggenstein, BESSY, Berlin, unpublished
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7. Examples of raytrace results

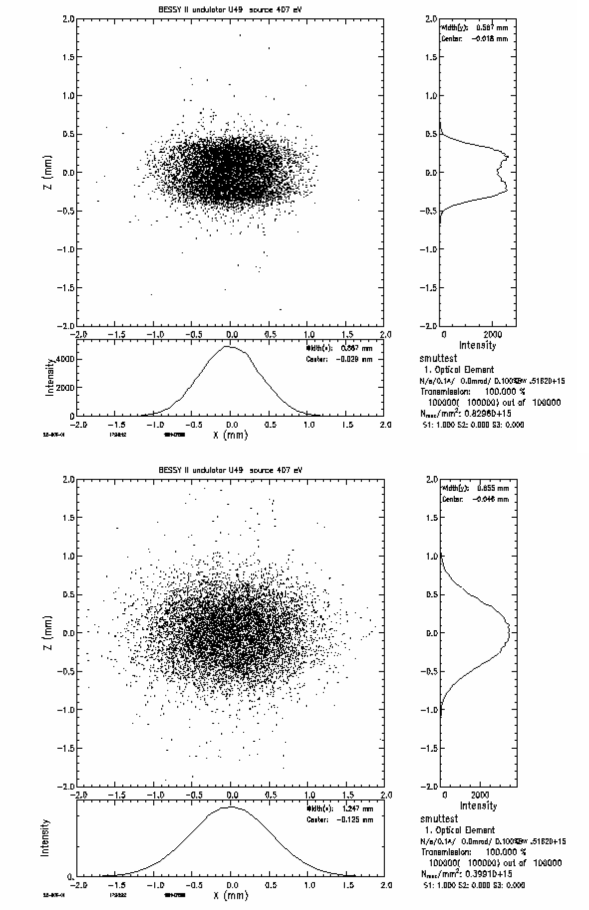

Figure 12 Spot patterns of the BESSY II undulator source U49 at 407 eV at 10 m downstream without (top) and with (bottom) electron beam emittance (σ_x/σ_y= 320/24 µm), source depth (4m), beam emittance (σ_x'/σ_y' =27/20 µrad)). The source data were calculated with SMUT /22/

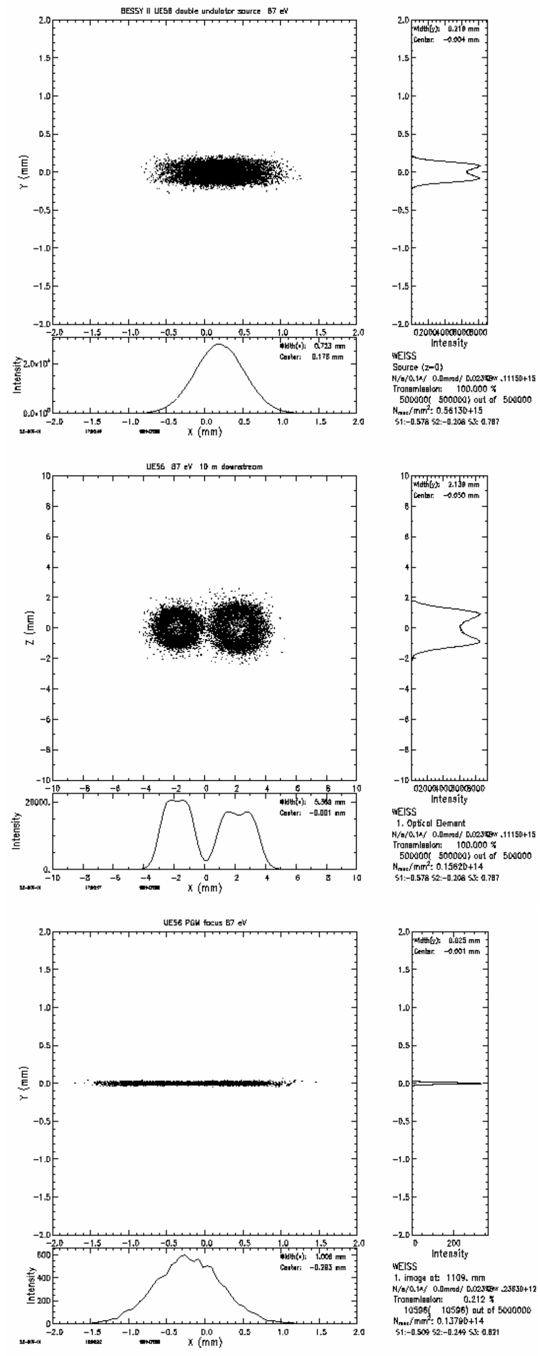

Figure 13 Spot patterns of the BESSY II double helical undulator source UE56 /15/ at 87 eV. *Top*: at the source (z=0); *Center:* 10 m downstream. The depth of field effect can be seen; *Bottom:* at the focus position of the UE56-Plane

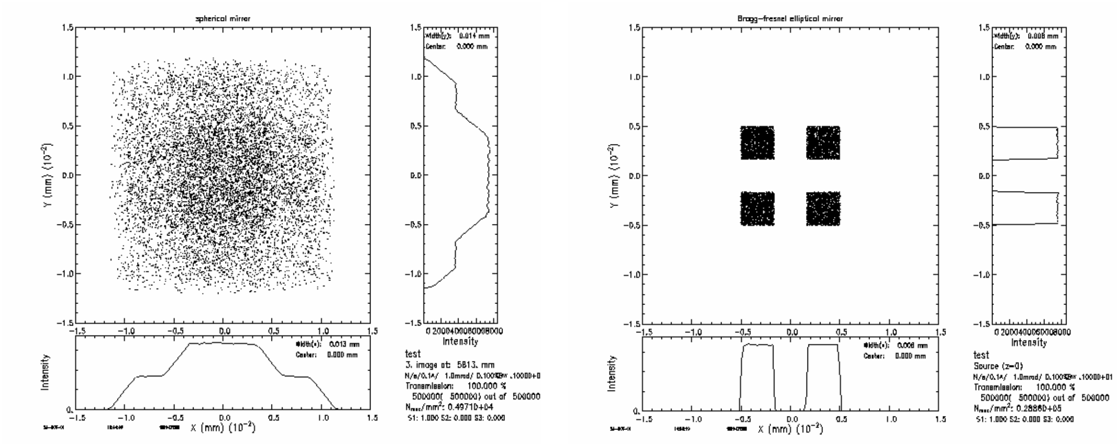

Figure 14 Normal incidence imaging of a test object of 3 µm x 3 µm squares (PI_XEL-source) with a spherical mirror (left) and with an elliptical Bragg-Fresnel lens (right) (taken from ref. 19). The spherical mirror does not reprocude the pattern because of its astigmatism.

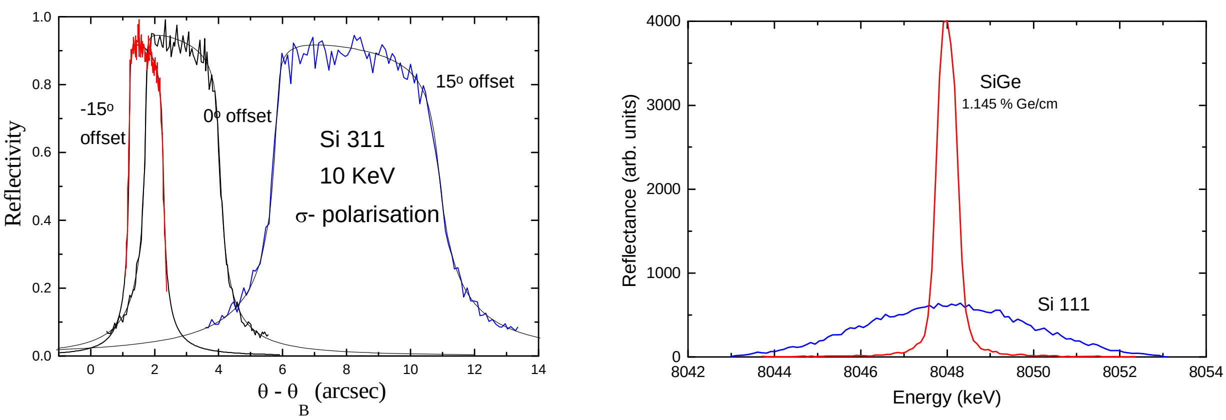

Figure 15 Crystal optics in *RAY*: left side: Comparison of Si (311) rocking curves at 10 keV for asymmetrical crystals (0, +/-15° offset) using *RAY* and the code DIXI (taken from ref 11).
right side: Energy resolution for a pure Si (111) crystal and a laterally graded SiGe-crystal (10° offset angle) at 8 keV. (taken from ref. 20).

8. Appendices

A1. Analytical geometry for pedestrians

Reference: Eric W. Weisstein. "Quadratic Surface." From *MathWorld*--A Wolfram Web Resource.
http://mathworld.wolfram.com/QuadraticSurface.html

A second-order algebraic surface given by the general equation

$$a x^2 + b y^2 + c z^2 + 2 f y z + 2 g z x + 2 h x y + 2 p x + 2 q y + 2 r z + d = 0. \tag{1}$$

Quadratic surfaces are also called quadrics, and there are 17 standard-form types. A quadratic surface intersects every plane in a (proper or degenerate) conic section. In addition, the cone consisting of all tangents from a fixed point to a quadratic surface cuts every plane in a conic section, and the points of contact of this cone with the surface form a conic section (Hilbert and Cohn-Vossen 1999, p. 12).

Define

$$e = \begin{bmatrix} a & h & g \\ h & b & f \\ g & f & c \end{bmatrix} \tag{2}$$

$$E = \begin{bmatrix} a & h & g & p \\ h & b & f & q \\ g & f & c & r \\ p & q & r & d \end{bmatrix} \tag{3}$$

$$\rho_3 = \operatorname{rank} e \tag{4}$$

$$\rho_4 = \operatorname{rank} E \tag{5}$$

$$\Delta = \det E, \tag{6}$$

and k_1, k_2, as k_3 are the roots of

$$\begin{vmatrix} a-x & h & g \\ h & b-x & f \\ g & f & c-x \end{vmatrix} = 0. \tag{7}$$

Also define

$$k \equiv \begin{cases} 1 & \text{if the signs of nonzero } k\text{s are the same} \\ 0 & \text{otherwise.} \end{cases}$$

Then the following table enumerates the 17 quadrics and their properties (Beyer 1987)

Surface	Equation	ρ_3	ρ_4	$\operatorname{sgn}(\Delta)$	k
Coincident planes	$x^2 = 0$	1	1		
Ellipsoid (Imaginary)	$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = -1$	3	4	+	1
ellipsoid (Real)	$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$	3	4	-	1
Elliptic Cone (Imaginary)	$\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = 0$	3	3		1

elliptic cone (Real)	$z^2 = \frac{x^2}{a^2} + \frac{y^2}{b^2}$	3	3		0
Elliptic Cylinder (Imaginary)	$\frac{x^2}{a^2} + \frac{y^2}{b^2} = -1$	2	3		1
elliptic cylinder (Real)	$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$	2	3		1
elliptic paraboloid	$z = \frac{x^2}{a^2} + \frac{y^2}{b^2}$	2	4	-	1
hyperbolic cylinder	$\frac{x^2}{a^2} - \frac{y^2}{b^2} = -1$	2	3		0
hyperbolic paraboloid	$z = \frac{y^2}{b^2} - \frac{x^2}{a^2}$	2	4	+	0
hyperboloid of one Sheet	$\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = 1$	3	4	+	0
hyperboloid of two Sheets	$\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = -1$	3	4	-	0
Intersecting Planes (Imaginary)	$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 0$	2	2		1
Intersecting planes (Real)	$\frac{x^2}{a^2} - \frac{y^2}{b^2} = 0$	2	2		0
parabolic cylinder	$x^2 + 2rz = 0$	1	3		
Parallel Planes (Imaginary)	$x^2 = -a^2$	1	2		
Parallel planes (Real)	$x^2 = a^2$	1	2		

Of the non-degenerate quadratic surfaces, the elliptic (and usual) cylinder, hyperbolic cylinder, elliptic (and usual) cone are ruled surfaces, while the one-sheeted hyperboloid and hyperbolic paraboloid are doubly ruled surfaces.

A curve in which two arbitrary quadratic surfaces in arbitrary positions intersect cannot meet any plane in more than four points (Hilbert and Cohn-Vossen 1999, p. 24).

Literature:

1. Beyer, W. H. CRC Standard Mathematical Tables, 28th ed. Boca Raton, FL: CRC Press, pp. 210-211, 1987
2. Hilbert, D. and Cohn-Vossen, S. "The Second-Order Surfaces." §3 in Geometry and the Imagination. New York: Chelsea, pp. 12-19, 1999.
3. Mollin, R. A. Quadrics. Boca Raton, FL: CRC Press, 1995.

A2. Source-Parameter buffer SPARAM(30)

	Source type Parameter	**MA**	**PO**	**PI**	**CI**	**DI**	**WI**	**WU**	**HU**	**UF**	**HF**	**FI**
1	no of succesful rays	x	x	x	x	x	x	x	x	x	x	x
2	no of source-type	1	2	3	4	7	8	9	10	11	12	13
3	source width (w_x / σ_x) (mm)	x	x	x	x	x	x	x	x	x	x	-
4	source height (w_x / σ_x) (mm)	x	x	x	x	x	x	x	x	x	x	-
5	source depth (w_z) (mm)	x	x	x	x	cal	cal	period	w_{z1}	x	w_{z1}	-
6	diverg. hor. (φ / σ_φ) (mrad)	x	x	x	no-ci	x	x	x	x	x	x	-
7	diverg. vert. (ψ / σ_ψ) (mrad)	x	x	x	φ_{max}	-	-	x	x	x	x	-
8	beam emittance σ_x’ (μrad)	-	-	-	φ_{min}	-	x	-	-	x	x	-
9	beam emittance σ_y’ (μrad)	-	-	-	$\Delta\varphi$	x	x	-	-	x	x	-
10	electron energy (GeV)	-	-	-	-	x	x	x	-	-	-	-
11	k-parameter	-	-	-	-	-	x	x	-	-	-	-
12	bending radius (m) / no. period	-	-	-	-	R	#per	#per	-	-	-	-
13	photon energy E (eV)	x	x	x	x	x	x	x	x	x	x	x
14	ΔE (eV) (+: discrete / -:cont.)	x	x	x	x	x	x	x	x	x	x	x
15	----	-	-	-	-	-	-	-	-	-	-	-
16	Stokes vector S_0 (flux)	1	1	1	1	cal	cal	cal	cal	cal	cal	1
17	Stokes vector S_1	x	x	x	x	cal	x	x	x	x	x	x
18	Stokes vector S_2	x	x	x	x	cal	x	x	x	x	x	x
19	Stokes vector S_3	x	x	x	x	cal	x	x	x	x	x	x
20	Pathlength (mm)	x	x	x	x	x	x	x	x	x	x	x
21	hor. inclination (U1) (mrad)	-	x	-	-	x	x	-	x	x	x	-
22	vert. inclination (U1) (mrad)	-	x	-	-	x	x	-	x	x	x	-
23	hor. inclination of U2 (mrad)	-	-	-	-	-	-	-	x	-	x	-
24	vert. inclination of U2 (mrad)	-	-	-	-	-	-	-	x	-	x	-
25	source depth U2 w_{z2} (mm)	-	-	-	-	-	-	-	x	-	x	-
26	offset in x-dir. (z f. U1) (mm)	-	x	-	-	x	x	-	x	x	x	-
27	offset in y-dir. (z f. U2) (mm)	-	x	-	-	x	x	-	x	x	x	-
28	option (U1/U2/both)	-	-	-	-	-	-	-	x	-	x	-
29	flag (U1/U2)	-	-	-	-	-	-	-	cal	-	cal	-
30	SMUT/WAVE-input file	-	-	-	-	-	-	-	-	x	x	-

x:	input parameter
cal:	buffer used and calculated in *RAY*
1,2,...:	buffer used with a fixed value
per, w_{z1},...	input parameter with different meaning

last update: 4. Jan. 2006

A3. Mirror-Parameter buffer MPARAM(10,60)

	Optical element Parameter	**SL**	**FO**	**ZO**	**PM**	**CY**	**CO**	**SP**	**TO**	**EL**	**PA**	**EP**	**ET**	**EO**	**PG**	**SG**	**TG**	**CR**	**CC**
1	no. of successful rays	calc	calc	calc	calc	calc	calc	calc	calc	calc	calc	calc	calc	calc	calc	calc	calc	calc	calc
2	no. of optical element	1	2	3	11	12	13	14	15	16	17	18	19	20	21	22	23	31	32
3	width / radius x / r_{min} (mm)	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
4	length(height)/ ra z/y/r_{max}(mm)	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
5	sag. entrancearm/b.stop x (mm)	stop	-	x	-	-	-	-	x	-	-	-	x	x	-	-	x	-	-
6	sag. exit arm/beamstop y (mm)	stop	-	X	-	-	-	-	x	-	-	-	x	x	-	-	x	-	-
7	mer entrance armlength (mm)	-	-	wlo	-	x	x	x	x	x	x	x	x	x	x	x	x	-	x
8	merid. exit arm length (mm)	-	-	F	-	x	x	x	x	x	col	col	x	x	-	x	x	-	x
9	grazing incidence angle (deg)	-	x	-	x	x	x	x	x	x	x	x	x	x	α /		($\alpha+\beta$)	x	x
10	radius R, along z (mm)	-	-		-	x	x	x	x	A	P	P	A	a_{11}	-	x	x	-	x
11	radius ρ, along x (mm)	-	-	-	-	x	x	-	x	B	-	-	B	a_{22}	-	-	x	-	x
12	rotfig. (a11) / fixfocus	-	-	-	-	-	-	-	-	C	C	-	ρ	a_{12}	c_{ff}	c_{ff}	E_{opt}	offs	offs
13	grating line density (l/mm)	-	-		-	-	-	-	-	α	-	-	α	a_{13}	x	x	x	d	d
14	diffraction order	-	-		-	-	-	-	-	-	-	-	-	a_{23}	x	x	x	V_c	V_c
15	1. lattice constant	-	-	-	-	-	-	-	-	-	-	-	-	a_{14}	-	-	-	x	x
16	2. lattice constant	-	-	-	-	-	-	-	-	-	-	-	-	a_{24}	-	-	-	x	x
17	grazing inc. angle α_{gr} (rad)	-	x	-	calc	calc	calc	calc	calc	calc	calc	calc	calc	x	calc	calc	calc	x	x
18	grazing exit angle β_{gr} (rad)	-	-	-	calc	calc	calc	calc	calc	calc	calc	calc	calc	x	calc	calc	calc	x	x
19	azimuthal angle χ (°)	-	x	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
20	misalignment $\delta\phi$ (mrad)	-	-	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
21	misalignment $\delta\psi$ (mrad)	-	-	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
22	misalignment $\delta\chi$ (mrad)	-	-	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
23	distance to prec. OE (mm)	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
24	misalignment δx (mm)	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
25	misalignment δy (mm)	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
26	misalignment δz (mm)	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
27	RMS tang.-error x-y ($\delta\chi$) (″)	-	-	-	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-
28	RMS tang. error y-z ($\delta\psi$) (″)	-	-	-	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-
29	atomic weight substrate	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
30	VLS-par. / CR-gradient	-	-	-	-	-	-	-	-	-	-	-	-	-	b_2	b_2	b_2	b_2	b_2
31	VLS-par. / disp. corr. inc.angle	-	-	-	-	-	-	-	-	z_0	-	z_0	z_0	α	b_3	b_3	b_3	x	x
32	VLS-par. / disp. corr. exit ang.	-	-	-	-	-	-	-	-	a_{33}	-	-	-	a_{33}	b_4	b_4	b_4	x	x
33	VLS-par./ CR-Miller index	-	-	-	-	-	-	-	-	a_{34}	-	-	-	a_{34}	b_5	b_5	b_5	h	h
34	VLS-par./ CR-Miller index	-	-	-	-	-	-	-	-	a_{44}	a_{44}	-	-	a_{44}	b_6	b_6	b_6	k	k
35	VLS-par./ CR-Miller index	-	-	-	-	-	-	-	-	y_0	y_0	y_0	y_0	isig	b_7	b_7	b_7	l	l
36	number of layers	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-
37	thickness substrate (nm)	-	x	x	-	-	-	-	-	-	-	-	-		-	-	-	-	-
38	thickness odd (1...) layers (nm)	-	x	-	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-
39	thickness even (2.) layers (nm)	-	x	-	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-
40	thickness top layer (nm)	-	x	-	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-
41	thermal / cyl.bow. amp. (μm)	-	-	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
42	th b. σ_x (μm) / bowing R (km)	-	-	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
43	thermal bump width σ_z (μm)	-	-	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
44	atomic weight 1. layer	-	x	X	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
45	profile (1/2/3/4) / struct. factor	-	-	-	-	-	-	-	-	-	-	-	-	b_{12}	x	x	x	F_o	F_o
46	blaze angle (°)/Efficiency / st-f	-	-	-	-	-	-	-	-	-	-	-	-	b_{21}	x/ef	x/ef	x/ef	F_o	F_o
47	aspect angle (°) / struct. factor	-	-	-	-	-	-	-	-	-	-	-	-	b_{13}	x	x	x	F_h	F_h
48	groove depth (nm) / struct. f.	-	-	-	-	-	-	-	-	-	-	-	-	b_{31}	x	x	x	F_h	F_h
49	groove width/spacing / struct.f.	-	-	-	-	-	-	-	-	-	-	-	-	b_{23}	x	x	x	F_{hc}	F_{hc}
50	structure factor	-	-	-	-	-	-	-	-	-	-	-	-	b_{32}	-	-	-	F_{hc}	F_{hc}
51	roughness substrate (nm)	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-

52	roughness odd layers (nm)	-	x	-	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-
53	roughness even layers (nm)	-	x	-	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-
54	roughness top layer (nm)	-	x	-	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-
55	density substrate (g/cm^3)	-	x	X	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-
56	density odd layers (g/cm^3)	-	x	-	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-
57	density even layers (g/cm^3)	-	x	-	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-
58	density top layer (g/cm^3)	-	x	-	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-
59	atomc weight 2. layer	-	x	-	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
60	atomic weight top layer	-	x	-	x	X	x	X	x	x	x	x	x	X	x	x	x	x	x
61	ML-gradient B1 (x**1)				x	x	x	x	x	x	x	x	x	x					
62	ML-gradient B2 (x**2)				x	x	x	x	x	x	x	x	x	x					
63	ML-gradient B3 (x**3)				x	x	x	x	x	x	x	x	x	x					
64	ML-gradient B4 (x**4)				x	x	x	x	x	x	x	x	x	x					
65	ML-gradient B5 (z**1)				x	x	x	x	x	x	x	x	x	x					
66	ML-gradient B6 (z**2)				x	x	x	x	x	x	x	x	x	x					
67	ML-gradient B7 (z**3)				x	x	x	x	x	x	x	x	x	x					
68	ML-gradient B8 (z**4)				x	x	x	x	x	x	x	x	x	x					
69																			
70																			
71																			
72																			
73																			
74																			
75																			
76																			
77																			
78																			
79																			
80																			

last update: 4.1.2006

A4. General Parameter buffers

a) Byte-parameter buffer BPARAM(1600)

		Name	Filename coating/ crystal	Mis align-ment y/n	Sur face profile y/n	Surface profile filename	Name odd layers	Name even layers	Name top layers	Not used
1	**Source**	1-2	4-23	-	-	-	-	-	-	34-80
2	**Optical element # 1**	81-82	84-99	101	103	104-112	113-128	129-144	145-160	-
3	**Optical element # 2**	161-162	164-179	181	183	184-192	193-208	209-224	225-240	-
	...	241-242	...	...	...	...	...	...	...	-
	...	...	...	...	...	...	...	...	...	-
11	**Optical element # 10**	801-802	804-819	821	823	825-832	833-848	849-864	865-880	-
12	**Image plane # 1**	881-882	-	-	-	-	-	-	-	883-960
13	**Image plane # 2**	961-962	-	-	-	-	-	-	-	963-1040
14	**Image plane # 3**	1041-1042	-	-	-	-	-	-	-	1043-1120
										1121-1440
	General information	**Par-file /User-name**	**Focusposition (y/n) / Date**				**Start-login-time**	**CPU-time**	**Ray-Version**	
		1441-1460	1500				-	-	-	1461-1499
	Entry in RAY.USER	1521-1532	1535-1543				1546-1553	1556-1567	1571-1600	1501-1520

b) Integer parameter buffer IPARAM(50)

1-14	----
15	# of test rays
16	no successful test rays
17	no of reflected test rays
18-20	----
21	no of optical elements (IM)
22	no of image planes (NIM)
23	1. image plane distance
24	2. image plane distance
25	3. image plane distance
26	search focus position at
27	+/-
28-29	----
30	parameter file (IPF)
31	no of turns (ITURN)
32-40	----
41	Plot device (IPLOT)
42	Hardcopy device (IHCP)
43-50	----

last update: 22. Dec 2005

A5. File Structure of the source-input file

The *RAY*-input file for the sources AS and HF is oriented along the output file of the undulator tracking codes *URGENT* /21/, *SMUT* /22/ or *WAVE* /23/. It is, however, not restricted to undulator radiation, but may contain any user-defined intensity pattern whatsoever. *RAY* interpretes the file contents as an intensity pattern of a point source at a distance of 10 m. The intensity is interpreted as photon flux/s/100 mA/0.1% bandwidth/pixel area. Only one quadrant of the total intensity distribution is given, *RAY* creates the full 4-quadrant emission spectrum by imaging this pattern along the x- and y-axes. The source volume and the beam emittance are taken into account by a convolution with this (single-electron) emission pattern. The number of pixels in the x- and y-directions are given in line 1 of the file, the pixel size is determined by the x- and y-coordinates of the pattern, given in mm at 10 m distance from the source.

1. line (n_x,n_y)	17,32
2. line (x,y,intensity)	0.000000e+00, 0.000000e+00, 1.102871e+12
3. line	1.843063e-01, 0.000000e+00, 2.219303e+12
...	3.686125e-01, 0.000000e+00, 1.533809e+12
...	5.529188e-01, 0.000000e+00, 7.595799e+10
...	7.372251e-01, 0.000000e+00, 2.896673e+09
	9.215313e-01, 0.000000e+00, 9.263270e+08
	1.105838e+00, 0.000000e+00, 5.743191e+07
......	
	2.764594e+00, 0.000000e+00, 1.917974e+08
(n_x+1). line	2.948900e+00, 0.000000e+00, 1.875684e+07
(n_x+2). line	0.000000e+00, 5.232785e-02, 1.198062e+12
	1.843063e-01, 5.232785e-02, 2.309749e+12
...	3.686125e-01, 5.232785e-02, 1.454328e+12
...	5.529188e-01, 5.232785e-02, 1.374431e+10
......	
(n_x x n_y)+1. line	3.041053e+00, 1.622163e+00, 7.742964e+09
end of file	

File structure for the Source input file U49_407EV.DAT

A6. File Structure of the surface profile file

The *RAY*-input file routine for the surface profile of optical elements matches the file structure of the ZEISS profile-measuring machine *M400* /27/. It can, however, be used for any kind of user-defined surface: e.g. a calculated profile using a finite element (FE) analysis program like *ANSYS* /24/. In this way implications connected with thermal load or mechanical stress problems by mirror bending techniques on the optical performance can be studied.
RAY interpretes the file as the distorted 2-dimensional height profile (n_x lines, n_z rows) of an optical element, i.e. the shape (cylindrical, ellipsoidal, etc...) is unaffected by the file-content. For a ray to be distorted by such a real surface the local slope at the intersection point is calculated by interpolation between the nearest neighbour points of the input surface mesh. Then the normal vector is rotated according to this slope error (in *x*- and *z*-direction), so that the reflected/diffracted ray changes direction adequately.
The local amplitude is NOT taken into account in the calculation.

The first line in the file contains the number of surface points n_x, n_z, ($n_{xmax} = n_{zmax}$ =251) and the distance between the points d_x, d_z, (units for ANSYS-profiles in mm, for ZEISS-profiles in nm). The rest of the file contains the amplitudes (*y*-coordinates in mm), starting with the *z*-direction (constant *x* values).
The width of the optical element is then to be $(n_x\text{-}1)\cdot d_x$ and the length $(n_z\text{-}1)\cdot d_{z.}$ The mirror center is at position *(nx/2+1/nz/2+1).*
For ZEISS-profiles the unit is nm, for ANSYS the input-amplitudes are interpreted as being in mm.

1. line (n_x,n_z,d_x,d_z)	30 30 0.689655 5.517241
2. line (y-amplitude at -z_{max},+x_{max}) .	-0.0001602439
3. line(y-amplitude at -z_{max}+d_z,+x_{max})	-0.0001243564
...	
...	
...	
(nz+1). line (y-amplitude at +z_{max},+x_{max})	-0.0001532434
(nz+2). line (y-amplitude at -z_{max},+x_{max}-d_x)	-0.0001169811
(nz+3). line (y-amplitude at -z_{max}+d_z,+x_{max}-d_x)	-0.0000859142
...	
...	
...	
($n_x \cdot n_y$). line (y-amplitude at z_{max}-d_z,-x_{max})	-0.0001243564
($n_x \cdot n_y$)+1. line (y-amplitude at z_{max},-x_{max})	-0.0001602440
end of file	

File structure for the *ANSYS*-surface profile input file U49_PGM.DAT

It contains the deformation of the first (SiC-) mirror in the BESSY-II U49-PGM-beamline at a k-parameter of 2.5 for 400 mA ringcurrent.

A7. File-structure of the RAY-parameter file YOURNAME.RAY

```
***********************************************************************

  RAYTRACE-PARAMETER FILE:                         toroid.RAY

  SCHAEFERS         11-SEP-97    10:11:05             RAY VERSION 23.4
***********************************************************************

     DI        1
     TO

  *********   Source parameters (SPARAM(30)     *********

  20000.0000000000        6.00000000000000        5.000000000000000E-002
 9.300000000000000E-002   1.00000000000000        1.000000000000000E-003
 1.000000000000000E-003  1.900000000000000E-005  1.300000000000000E-005
  1700.00000000000       0.000000000000000E+000   4350.00000000000
  10.0000000000000       0.000000000000000E+000   1394148006744.70
 0.000000000000000E+000  -1.00000000000000        0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000

  *********    OE parameters (MPARAM(IM,50)     *********

 0.000000000000000E+000   5.00000000000000        -100.000000000000
  100.000000000000       -500.000000000000         600.000000000000
  20000.0000000000        1000.00000000000         160.000000000000
  10969.0866345593        330.758433651296        0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000  0.174532925199433        0.174532925199433
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000   20000.0000000000        0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000  1.123430852883921E-153  0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000  1.607123823107359E+256
 0.000000000000000E+000   1.28259813785553        0.987146496772766
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000  1.123430852883921E-153  0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000

  *********  General parameters (IPARAM(100))  *********

  538986820   538988372   538987849   538976288   538976288   538976288
  538976288   538976288   538976288   538976288   538976288           0
          0           0           0           0           0           0
          0           0           1           1        1000        1000
       1000        1000         100           0           0           2
          1           0           0           0           0           0
          0           0           0           0          51          61
          0           0           0           0           0           0
          0           0        2000           0           0           0
          0           0           0           0           0           0
          0           0           0           0           0           0
          0           0           0           0           0           0
          0           0           0           0           0           0
          0           0           0           0           0           0
          0           0           0           0           0           0
          0           0           0           0           0           0
          0           0           0           0
```

Position Limits at Source (X-Y),Opt. Elements (X-Z) (mm)
and Image Planes (X-Y) :

No	Name	Xmin	Xmax	Y(Z)min	Y(Z)max
1:	DI	-0.1488	0.1492	-0.2768	0.2576
2:	TO	-10.1697	10.0511	-499.5712	564.2416
3:	IM	-3.1255	3.9207	-40.4978	0.0065

No	Name	PHI_min	PHI_max	PSI_min	PSI_max
1:	DI	-0.0315	0.0316	-0.3220	0.3453
2:	TO	-0.7363	0.7753	73.8907	85.5525
3:	IM	-0.7363	0.7753	-5.5321	6.1214

1968 rays successful out of 2000 rays

No of successful/reflected Rays, Reflectance,Flux density and Flux
at Source, Opt. Elements and Image Planes:

No	Name	N_geometric	N_reflected	Max. Flux density (N/mm**2)	Flux (N/s/0.1A/ 0.10%BW)
1:	DI	20000.	20000.	0.875422D+14	0.139415D+13
2:	TO	19686.	14756.	0.291480D+09	0.102860D+13
3:	IM	19686.	14756.	0.283769D+13	0.102860D+13

No	Name	Stokes-Vector: S0	S1/S0	S2/S0	S3/S0
1:	DI	1.00000	-1.00000	0.00000	0.00000
2:	TO	0.75102	-1.00000	0.00000	0.00000
3:	IM	0.75048	-1.00000	0.00000	0.00000

****

RAYTRACE-PARAMETER FILE: toroid.RAY
SCHAEFERS 11-SEP-97 10:11:05 RAY VERSION 23.4

****

A8. Example for a RAY-session: Interactive input of parameters

```
SCHAEFERS_BESSY-I_VAX> r prg:ray



                  ######          #        #       #
                  #     #        # #        #     #
                  #     #       #   #        #   #
                  ######       #     #        # #
                  #   #        #######         #
                  #    #       #     #         #
                  #     #      #     #         #




***********************************************************************
                                WELCOME TO

                                R   A   Y

                       THE BESSY RAYTRACE PROGRAM

                       Version 23.4 of FEB. 17, 1997

                       Franz Schaefers,  BESSY mbH
                       Lentzeallee 100, D-14195 BERLIN
                       Tel. +49-(0)30-82 004-162
                       FAX                   -149
                       e-mail SMTP: schaefers@exp.bessy.de

***********************************************************************
                                                               <RETURN>


Info ?    (Y/N)                          [   NO  ] :
Use PARAMETER FILE ?       (Y/N)         [  YES  ] :n
Which TERMINAL are you using? (EXIT=99)
               VT100                    = 1
               VISUAL                   = 2
               X-Window (DEC-Term)      = 3
               X-TERM                   = 5
               NO GRAPHIC (BATCH-JOB)   = 6 [    3  ] :

HARDCOPY ON:
     -- cancel/ignore (no hardcopy)      =  0
     -- POSTSCRIPT (PS)-PRINTERS:
            RAY_PRINTER_PS1              =  1
            RAY_PRINTER_PS2              =  2
     -- PS- FILE on your login-directory =  3
     -- EPS-FILE on your login-directory =  4
     -- Help ?                           = 99  [    1  ] :

How many rays ?                  [     50000.    ] :20000.


Source type:           MA__trix (hard edge and ang. distr.)
```

```
                       PO__int  (hard edge and ang. distr.)
                       PI__xel  (hard edge and ang. distr.)
                       LI__ne   (gaussian edge and ang. distr.)
                       HL__ine  (hard edge, gaussian ang. distr.)
                       CO__ne   (hard edge and ang. distr.)
                       DI__pole (gaussian edge, hard hor. ang. distr.)
                       WI__ggler (gaussian edge)
                       WU__Wiggler/Undulator (gauss. edge, hard ang.distr.)
                       FI__le (ASCII-Data-file)       [   DI  ] :

Source width
  (MA,PO,CO,HL:hard; LI,DI:sig-x)[   0.05000  mm ] :
Source height
  (MA,PO,CO,HL:hard; LI,DI:sig-y)[   0.09300  mm ] :
Horiz. divergence
  (MA,PO,DI:hard; LI,HL:sig.-phi)[     1.000 mrad] :
Electron energy                  [  1700.000 MeV ] :
Bending radius                   [  4350.000  mm ] :
    Magnetic Field Strength B0   [     1.303  T  ]
    Critical Energy              [     2.505 keV ]
Photon energy (Total Power: =0)  [   100.000  eV ] :10.
  (Photon wavelength   123.985 nm)
+/-Delta-E ? (<0:cont, >0:discr) [   0.00000  eV ] :
Linear polarization (S1/S0)      [    -1.000     ] :
Linear polarization (S2/S0)      [     0.000     ] :
Circular polarization (S3/S0)    [     0.000     ] :
   ....Total polarization :      [     1.000     ]

O.K. ?   (Y/N)                              [  YES  ] :
PHOTON FLUX:0.1394D+13 /sec/100mA/ 1.0mrad/ 0.100%BW

How many optical elements ?  (0-10)      [   1   ] :

  1. optical Element   SL__it
                       FO__il
                       ZO__neplate
                       PM__plane mirror
                       CY__linder (X- or. Z-dir.)
                       CO__ne (Z-dir.)
                       TO__roidal (spherical) mirror
                       PA__raboloid
                       EL__lipsoid
                       EP__elliptical paraboloid
                       PG__plane grating
                       TG__toroidal (spherical) grating
                       CR__ystal                        [   PM  ] : TO

Mirror(slit,grating) size: X(R)_min[ -100.0000 mm] :
                          :X(R)_max[  100.0000 mm] :
     (for slit: Y_min)    :  Z_min [ -500.0000 mm] :
     (for slit: Y_max)    :  Z_max [  600.0000 mm] :
Distance source-opt.element        [      10.0 mm] :20000.
Distance opt.element-focus         [    10.000 mm] :1000.
Total deviation                    [179.0000degr.] :160.
   (calculated R =   10969.1 mm)
Long radius R (par. ray) (0=plane) [    10969. mm] :
   (calculated rho =    330.76 mm)
Short radius rho (0=plane)         [     330.8 mm] :
Distance zq to preceding element   [ 10000.000 mm] :20000.
Azimuthal angle (V:0,180, H:90,270)[     0.000deg] :
Name of Coating/Foil/Crystal       [ Au          ] :
   reading opt.const.-file: Au.nkp   (      5 -    9919 eV    301 points)
   density (calcul. from atomic data)   19.300 g/cm^3
Misalignment or Surface Errors ? (Y/N)  [   N   ] :
O.K. ?   (Y/N)                              [  YES  ] :
Display beam-width / z (determine focus)?[  NO   ] :y
search in a distance fr. last OE of[  1000.000 mm] :
```

```
            ... +/-                [   100.000 mm] :
How many point diagrams ? (1-3)    [         1   ] :
1. image distance for p.- diagram  [  1000.000 mm] :
Write parameters to file ? (Y/N)         [   NO  ] :y
Filename?  (without ext.)    [                     RAY] :toroid
Data stored in file ******                   toroid.ray ******
      raytracing test loop #         200
      raytracing test loop #         400
      raytracing test loop #         600
      raytracing test loop #         800
      raytracing test loop #        1000
      raytracing test loop #        1200
      raytracing test loop #        1400
      raytracing test loop #        1600
      raytracing test loop #        1800
      raytracing test loop #        2000



Position Limits at Source (X-Y),Opt. Elements (X-Z) (mm)
and Image Planes (X-Y) :

  No   Name        Xmin          Xmax         Y(Z)min       Y(Z)max

  1:    DI       -0.1488        0.1492        -0.2768        0.2576
  2:    TO      -10.1697       10.0511      -499.5712      564.2416
  3:    IM       -3.1255        3.9207       -40.4978        0.0065

  No   Name      PHI_min       PHI_max        PSI_min       PSI_max

  1:    DI       -0.0286        0.0286        -0.2918        0.3135
  2:    TO       -0.6678        0.7033        74.4196       84.9972
  3:    IM       -0.6678        0.7033        -5.0036        5.5665

              1968 rays successful out of  2000 rays



change limits ?            (Y/N)         [   NO  ] :
      Plot Focus Position:
xmin   ?                 [      891.00000 ] :
xmax   ?                 [     1109.00000 ] :
ymin   ?                 [        3.69111 ] :
ymax   ?                 [       42.74496 ] :
Header ?            [ ] : toroid focusposition
      change scale ?              (Y/N)  [   NO  ] :
      hardcopy ? (Y/N)                   [   NO  ] :
1. image distance for p.- diagram  [  1000.000 mm] :

start with raytracing ?    (Y/N/E_xit)   [  YES  ] :

     raytracing at ray number:    2000.      (CTRL/H: finish, CTRL/K: stop)
     raytracing at ray number:    4000.      (CTRL/H: finish, CTRL/K: stop)
     raytracing at ray number:    6000.      (CTRL/H: finish, CTRL/K: stop)
     raytracing at ray number:    8000.      (CTRL/H: finish, CTRL/K: stop)
     raytracing at ray number:   10000.      (CTRL/H: finish, CTRL/K: stop)
     raytracing at ray number:   12000.      (CTRL/H: finish, CTRL/K: stop)
     raytracing at ray number:   14000.      (CTRL/H: finish, CTRL/K: stop)
     raytracing at ray number:   16000.      (CTRL/H: finish, CTRL/K: stop)
     raytracing at ray number:   18000.      (CTRL/H: finish, CTRL/K: stop)
     raytracing at ray number:   20000.      (CTRL/H: finish, CTRL/K: stop)


No of successful/reflected Rays, Reflectance,Flux density and Flux
at Source, Opt. Elements and Image Planes:
```

```
  No   Name  N_geometric N_reflected  Max. Flux density   Flux
                                        (N/mm**2)   (N/s/0.1A/ 0.10%BW)

  1:   DI      20000.      20000.     0.875422D+14     0.139415D+13
  2:   TO      19686.      14756.     0.291480D+09     0.102860D+13
  3:   IM      19686.      14756.     0.283769D+13     0.102860D+13

  No   Name  Stokes-Vector: S0     S1/S0        S2/S0        S3/S0

  1:   DI           1.00000     -1.00000      0.00000      0.00000
  2:   TO           0.75102     -1.00000      0.00000      0.00000
  3:   IM           0.75048     -1.00000      0.00000      0.00000

Display source ?                          [   NO  ] :
Display 1. optical element (TO) ?         [   NO  ] :
Display 1. image plane ?                  [   NO  ] :y
   Display point-diagram (footprint) ?   [   NO  ] :y
xmin   ?                [       -4.84242 ] :
xmax   ?                [        4.57991 ] :
ymin   ?                [      -45.06992 ] :
ymax   ?                [        4.10372 ] :
Header ?           [ ] : toroid image
      change scale ?             (Y/N)  [   NO  ] :
      hardcopy ? (Y/N)                  [   NO  ] :
      Store Footprint data ?     (Y/N)  [   NO  ] :
   Display vertical profile  (sum) ?    [   NO  ] :
   Display horizontal profile (sum) ?   [   NO  ] :
   Display energy distribution ?        [   NO  ] :
   Display hor. angular distribution  ? [   NO  ] :
   Display vert. angular distribution  ? [   NO  ] :
   Display 3-D intensity profile ?      [   NO  ] :
   Contour-Plot ? (< 4 minutes!)        [   NO  ] :
   store all data ?                     [   NO  ] :

Repeat graphics          (Y/N/E_xit) ?   [   NO  ] :e
Print par/log-file       (Y/N) ?         [   NO  ] :
FORTRAN STOP
SCHAEFERS_BESSY-I_VAX>
```