Development of software for design, optimization and operation of
X-ray compound refractive lens systems

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1 Introduction and motivation

The main aim of my work was to create a software package that can be used for designing a configuration of CRL-based (compound refractive lens) optics in accordance with:

- type of the experiment (make divergent/convergent/parallel beam)
- minimization of total amount and types of lenses
- maximization of photon flux after the optical system

The optimized design of the CRL optics should be capable of covering the working X-ray energy range from 15 keV to 35 keV

1.1 Construction of new beamlines of PETRA extension

The PETRA III extension project adds two new experimental halls on either side (North and East) of the existing “Max-von-Laue Hall” facilities making use of the long straight section and part of the adjacent arcs (Fig. 1.1.1).

![Figure 1.1.1. View of the PETRA III storage ring (red line). The present experimental hall is shown together with the planned additional experimental halls in the North and East.](image)

The northern straight section already accommodates one of two 40 m long damping wiggler arrays producing an extremely hard and powerful X-ray beam which will also be utilized for materials science experiments. The long straight section in the west is available for additional insertion devices. In order to accommodate insertion device sources in the arc sections, which were filled with long dipole magnets yielding a rather soft X-ray spectrum, the machine lattice will be modified. The new lattice adds double bent achromat (DBA) cells in the arcs, each allowing for a 5 m long straight section. Similar to the present PETRA III beamlines, these straights will serve two beamlines
independently by use of canting dipoles resulting in two separate 2 m long straights. Different from the present 5 mrad canting scheme, a canting angle of 20 mrad was chosen at the extension beamlines to provide more spatial flexibility for the experiments further downstream. In total, the new lattice provides eight short straight high-β sections in the two arcs making them very suitable for the use of undulators. Overall, 11 new beamlines will be built in different phases. Five of the new beamlines will be designed as "short undulator" beamlines continuing most of the productive techniques formerly provided at DORIS III bending magnet beamlines. These sources will not only be very well suited for the spectrum of applications to be relocated from DORIS III but also provide a considerably brighter beam. In addition, four high-brilliance long undulator beamlines will be built in PETRA III hall East, three of them in collaboration with international partners, Sweden, India and Russia.

1.2 Russian-German nanodiffraction beamline (P23) at PETRA extension

The main focus of the beamline will be on the application of in situ and in operando diffraction techniques for the study of low-dimensional and nanoscale systems, i.e. structural properties and especially their evolution during chemical processes or under non-ambient conditions, such as high pressure, low temperature, electrical and magnetic fields, laser irradiation etc.

Examples of scientific cases are:

**Space averaging methods**

The most common and demanded application of X-ray diffraction is conventional space averaging scattering from bulk and surface objects. One major focus lies on the investigation of catalytic processes and relevant materials. Conventional averaging X-ray diffraction techniques are e.g. being used for the investigation of atomic structure of surfaces. A large part of the in situ research is dedicated to liquid/solid interfaces, e.g. the growth of complex functional nanomaterials and their properties. Progress has especially been achieved in time-resolved investigations of phase transformations, such as crystallization of immobilized nanoparticles from the amorphous phase, electric field induced phase transitions and ferroelectric switching mechanisms.

**Diffraction microscopy of bulk objects**

Diffraction using X-ray microbeams has considerably widened the research possibilities at the nanoscale. This applies not only to novel nanoscaled objects, but also to investigations of already well-studied materials that can be re-visited with access to ultra-short length scales. The basic diffraction tomography analysis can be combined with X-ray fluorescence spectroscopy and XANES. Along with the phase analysis in complex polycrystalline structures, pencil beams are also used for the investigation of local strain tensors, stress and microstructure evolution in nanocrystalline materials. This technique is applicable to single crystals, composite and functional graded materials.

**Diffraction microscopy of nanosized objects**
Microbeam X-ray diffraction is gaining importance as an effective tool for studying single nanocrystalline objects and oriented arrays of such objects. Technically, the studies of individual objects at the nanoscale are very challenging and require, along with an extraordinary stability of the instrument and the X-ray optical system, a parallel application of state-of-the-art nano-sample handling and characterization techniques. Combination of microbeam diffraction with anomalous scattering to investigate distortions in scanning probe nanolithography demonstrated an opportunity to use nanoscale strain variations for the selection of the initial material state in ferroelectrics, dielectrics, and other complex oxides. Additional opportunities arise through the parallel use of atomic force microscopy which allows selective introduction of defects or simultaneous probing of elastic properties in single nanocrystals.

**Coherent diffraction imaging of nanosized objects**

Coherent Diffraction Imaging (CDI) can be applied to investigate two- and three-dimensional structures with a resolution at 10 nm scales. CDI has developed into a characterization method capable of observing also the inner structure of complex nanoparticles and measuring internal strain evolution in nanoparticles under extreme conditions.

**X-ray Bragg diffraction ptychography**

The advantages of CDI can be combined with the structural sensitivity of conventional X-ray diffraction which is utilized in Bragg Diffraction Ptychography (BDP). The BDP method was also shown to deliver detailed information on the strain field around single dislocations in silicon. With a focal spot as large as 1 μm, it was possible to resolve the strain with a resolution down to 50 nm. This value could be further improved by increasing the photon flux in the focal spot. BDP is a unique tool for the investigation of domain structures and domain wall configurations in complex ferroelectric and multiferroic thin film systems, which is hardly obtainable with any other method. Bragg diffraction ptychography is very relevant for the scientific case of the beamline. A constraint on its applicability could be the short focal length of the optics necessary to reach focal spots at the diffraction limit. However, improved methods of data evaluation with partially coherent beams could allow to overcome this condition and make it available for in situ measurements.

The following requirements were defined for the nanodiffraction beamline:

– It should implement X-ray diffraction based methods which make use of the high source brilliance and focus on in situ techniques, such as experiments under non-ambient conditions, time-resolved measurements and the investigation of growth processes and chemistry of low-dimensional and nanoscaled materials, as well as the study of functional materials in operando.

– Two separate experiment hutch should be available in an inline configuration, alternately sharing the beam from the undulator: one hutch for diffractometer based experiments and a second hutch for
accommodating rather large and complex instrumentation for sample growth and characterization including a UHV facility.

– The diffractometer must allow for heavy in situ sample environments for the investigation of growth, electrochemistry, chemical reactions, catalysis, etc.

– A set of dedicated sample cells should be developed for the beamline and be made available for user groups. The decision on the types of sample cells will be made later depending on user demand.

– The X-ray optics of the beamline should provide a high brilliance monochromatic beam in the energy range from 5 keV to 35 keV and a photon flux \(\sim 10^{13}\) photons/sec at 10 keV.

– The beam spot at the sample position should vary from \(\sim 0.3 \times 0.3\) mm\(^2\) down to sub-micrometer dimensions.

**1.3 Beamline layout.**

Beamline P23 will be located in Hall East (PXE) of the PETRA III Extension (Fig. 1.3.1), sharing the sector with the Nano X-ray spectroscopy beamline P22.

![Figure 1.3.1. Schematic beamline arrangement and detailed floor plan (insert) of Hall East](image)

Both undulators share the same straight section of the storage ring, beams are separated by a canting angle of 20 mrad. This proximity imposes some constraints on the geometrical configuration of the beamlines, both in the common X-ray optics hutch and the downstream experimental area. Beamline P23 will have a total length of 110 m and operate two endstations in two experimental hutches, EH1 (upstream) and EH2 (downstream). Both endstations share the same primary X-ray optics and will be operated alternately. The downstream hutch EH2 will be accessible during the operation of EH1, so that the instrumentation in EH2 can be used in off-line mode as well. The respective distances from the source are given in Table 1.4.1 and Figure 1.4.2. EH1 is 7.5 m long and 4 m wide, EH2 is 6.9 m long and 6.3 m wide. Control hutch one (CH1) is placed adjacent to EH1, while CH2 is placed above EH2 in order to gain additional floor space for the experiment. This option is not available for EH1 because of interference with the large crane servicing the optics hutch and frontend area.
2 Beamline optics

2.1 Necessary requirements to the beamline optics.

The following requirements for the beam parameters in nanoscale X-ray diffraction have been compiled:

- spot cleanliness. It is important to notice that high-resolution diffraction experiments are sensitive both to the spatial and angular distribution of the photons, in contrast to other techniques such as small angle X-ray scattering or chemical analysis microscopy.
- high stability against mechanical drifts and vibrations. To meet this requirement, demanding design efforts will be needed in case of in-situ sample environments and especially for heavy sample cells.
- focal distance. Long focal distances are very desirable not only to preserve a low beam divergence but also to leave sufficient space for larger sample environments. Obviously, longer distances lead to larger focal spot sizes and also additional challenges to handle stability issues.
- wavefront distortion for coherent beam experiments. The form of the incident wavefront is an important parameter in the data evaluation procedures used in coherent scattering methods. A complex wavefront profile that could arise due to optics imperfection can strongly impede the convergence of numerical evaluation procedures, while any instability in this parameter would in most case make the data evaluation completely impossible.
- maximal possible photon flux density in the focal spot.

Energy tunability and resolution at the beamline should be sufficient for XANES and resonant X-ray scattering measurements as well as for wavelength scans of Bragg reflections. The latter option can be, in many cases, a solution to the problem of sample displacements during angular scanning. The beamline optics must be designed to meet these requirements, but also to allow accommodation of further optical elements for future developments. The optical system should be reliably switchable between different configurations.

2.2 Beamline optics layout. Source properties

The focusing optics must provide focused beams at two endstations positioned in EH1 and EH2 at distances of ~88 m and ~108 m from the source. The targeted values of beam cross sections in different operation modes, as discussed above, vary from ~0.3 mm down to ~1 µm in an energy range from 4 keV to 35 keV. Smaller beams can be realized, but at the expense of reduced flux caused by limiting apertures.

It is planned to employ two main beam focusing schemes: mirror-based for energies below 15 keV and CRL-based for energies above 15 keV. There is a certain overlap of energy ranges optimal for both
approaches, which allows combined variants depending on the application. Moreover, at all energies the CRLs will be complemented with flat mirrors for harmonics suppression. The focusing elements close to the sample may also vary: for lower energies, KB systems will be preferably used. However, in some cases one might also utilize Fresnel zone plates, especially for ultra-compact and/or in-vacuum installations. For high energies, CRLs will be most effective and flexible for X-ray focusing. The distances between optical components and the source are summarized in Figure 17. Together with the source properties, they define the key parameters of possible optical configurations. There are also some specific technical boundary conditions that must be taken into account:

- it is not planned to use white beam mirrors in phase 1 of the beamline implementation. Therefore the mirror systems will be placed downstream of the monochromator.
- within the current generic frontend design it is not feasible to place larger optical components inside the ring tunnel. However, there is an option to insert water-cooled CRLs at ~43 m from the source.
- in the optics hutch, the P23 beam path runs close to the concrete shielding wall. For practical reasons, the closest position of the double-crystal monochromator (DCM) to the source is at 55 m.

The initial beam after undulator has sizes $FWHM_{hor} = 0.332 \text{ mm}$, $FWHM_{ver} = 0.012 \text{ mm}$. First focusing optics is installed at 60 m from undulator. Since beam is divergent (and divergence depend on energy of photons) its size shown at fig. 2.2.2.
Figure 2.2.2
3 Focusing with lenses

3.1 Basic facts: geometrical optics

The lens-maker formula for a lens made from material with a refractive index \( n \) with radii of curvature of surfaces \( R_1, R_2 \) and distance \( d \) between them reads as:

\[
\frac{1}{f} = (n - 1) \left( \frac{1}{R_1} - \frac{1}{R_2} + \frac{(n-1)d}{nR_1R_2} \right) \quad (3.1.1)
\]

For a convex \((R_1 > 0, R_2 < 0)\) thin lens \((d \ll |R_1|)\) with equal radii of curvature \( R \) on both sides eq. 3.1.1 transforms to:

\[
f = \frac{R}{2(n-1)} \quad (3.1.2)
\]

A refractive index:

\[
n = 1 - \delta + i\beta, \delta \sim 10^{-7} \div 10^{-5} > 0 \\
\beta = \frac{\lambda \mu}{4\pi} \quad (3.1.3)
\]

where \( \mu \ (mm^{-1}) \) – linear absorption coefficient, \( \lambda \) – wavelength of photons. Since the mass absorption coefficient decreases with atomic number \( Z \) like \( Z^3 \), the lens material is chosen to minimize absorption – e.g. aluminum or (even better) beryllium (fig. 3.1.1, right). On beamline P23 beryllium lenses will be used.

The real part of \( n \) for x-rays in any material is below 1 (for beryllium – fig. 3.1.1, left), it means that for converging x-ray lens \( R \) should be below zero, so the lens is concave (fig. 3.1.2) with focus:

\[
f = \frac{R}{2|\delta|} \quad (3.1.4)
\]

![Figure 3.1.1. Refractive index and absorption coefficient vs x-rays energy for Be (from XOP)](image)

In parabolic lens its surfaces are paraboloids of rotation given by:
\[ z = \frac{r^2}{2R} \]  

(3.1.5)

Here \( z \) lies on the optical axis, \( r \) is perpendicular to it. The single lenses are about \( l = 1 \, mm \) thick and have distance between parabolic surfaces \( d \approx 0.03 \, mm \) (fig. 3.1.2). So aperture radius \( R_0 \) depends on the radius of curvature of parabola \( R \) as:

\[ R_0 = \sqrt{(l - d)R} \]

*Figure 3.1.2. Parabolic lens*

For a beryllium lens with a radius 1.5 mm at 15 keV (\( \delta = 1.5 \cdot 10^{-6} \)) focus distance will be \( f = 1.5 \cdot 10^{-3}/2 \cdot 1.5 \cdot 10^{-6} \) = 500 m. Therefore, to reach smaller focuses it’s necessary to make a CRL. CRL with \( N \) individual lenses will have a focus:

\[ f_N = \frac{R}{2N\delta} \left( 1 + O(\delta) \right) \approx \frac{R}{2N\delta} \]

(3.1.6)

where the correction term (spherical aberration) is typically below \( 10^{-4} \). Due to the large depth of field of refractive X-ray lenses and due to the large distances from source to CRL, from sample to CRL and large focus distance, the correction can be neglected for all practical purposes and a parabolic CRL can be considered as free of spherical aberration [1].

A distance \( a \) between object and thin lens and distance \( b \) between lens and image are connected with focus \( f \) like:

\[ \frac{1}{f} = \frac{1}{a} + \frac{1}{b} \]

(3.1.7)

For a more common case of thick lens: \( a \) is distance from object to first principal plane and \( b \) – from second principal plane to image. Calculation of parameters for system made of only two thick lenses becomes quite difficult [2]. Another issue – equation (3.1.6) works only for one lens radius and number. If some different lens types appears in one transfocator it requires to consider them as some thick lenses. So, number of such thick lenses for system with two transfocators could reach 4-6 pieces. Therefor, using of “familiar” geometrical optics becomes very inconvenient.

Another way to calculate parameters of CRL is described in the part 3.2.
3.2 Coherent X-ray focusing. Ray transfer matrix analysis

Ray transfer matrix analysis is a type of ray tracing technique used in the design of laser optical systems. This technique uses the paraxial approximation of ray optics, which means that all rays are assumed to be at a small angle and a small distance relative to the optical axis of the system. It involves the construction of a ray transfer matrix \( M \) which describes the optical system; tracing of a light path through the system can then be performed by multiplying this matrix with a vector representing the light ray:

\[
\begin{pmatrix}
x_2 \\
a_2
\end{pmatrix} = M \begin{pmatrix}
x_1 \\
a_1
\end{pmatrix}, \quad M = \begin{pmatrix}
A & B \\
C & D
\end{pmatrix}
\]  \hspace{1cm} (3.2.1)

where \( x_1 \) and \( a_1 \), \( x_2 \) and \( a_2 \) – coordinate and angle of the beam on the entrance and on the exit of optical system respectively (Fig. 3.2.1).

![Figure 3.2.1. Schematic view of optical system](image)

For a thin lens with focal length \( f \) matrix looks like:

\[
M_L = \begin{pmatrix}
1 & 0 \\
-1/f & 0
\end{pmatrix}
\]  \hspace{1cm} (3.2.2)

For propagation on the distance \( d \) through a free space with refraction index \( n \) matrix is:

\[
M_S = \begin{pmatrix}
1 & d/n \\
0 & 1
\end{pmatrix}
\]  \hspace{1cm} (3.2.3)

To make a matrix of optical system it’s necessary to multiply all matrices of single elements in reverse order. It means that if there are elements (from left to the right) with matrices \( M_1, M_2, \ldots, M_N \) the matrix of optical system will be (see Figure 3.2.1):

\[
M = M_N \cdot \ldots \cdot M_2 \cdot M_1
\]  \hspace{1cm} (3.2.4)

Matrix approach allows to determine location of cardinal points of optical system through \( A, B, C, D \) coefficients. Some of them are:

- Principal point 1 (measured from the entrance of system):

\[
PP_1 = \frac{d-1}{c}
\]  \hspace{1cm} (3.2.5)
Principal point 2 (measured from the exit of system):

\[ PP_2 = \frac{1-A}{c} \] \hspace{1cm} (3.2.6)

Focal points (measured from corresponding principal points):

\[ F = -\frac{1}{c} \] \hspace{1cm} (3.2.7)

Another useful feature – matrix optics allows to investigate a propagation of Gaussian beams. It’s assumed that beam is coherent. Gaussian beam is characterized by complex beam parameter \( q \):

\[ \frac{1}{q} = \frac{1}{R} - \frac{\lambda}{\pi w^2} \] \hspace{1cm} (3.2.8)

here \( \lambda \) – wavelength of radiation, \( R \) – radius of curvature of wavefront:

\[ R(z) = z \left( 1 + \left( \frac{x_R}{z} \right)^2 \right), z_R = \frac{\pi w_0^2}{\lambda} \] \hspace{1cm} (3.2.9)

\( w \) – width of the beam (FWHM = \( w \cdot \sqrt{2 \cdot \ln(2)} \)):

\[ w(z) = w_0 \sqrt{1 + \left( \frac{x}{z_R} \right)^2} \] \hspace{1cm} (3.2.10)

where \( z_R \) – Rayleigh range, \( w_0 \) – beam waist (minimal value of beam width).

When beam passes an optical system beam parameter changes by the “ABCD rule”:

\[ \frac{1}{q_2} = \frac{C+D/q_1}{A+B/q_1} \] \hspace{1cm} (3.2.11)

Using this rule one can calculate new beam size and new radius of curvature of wavefront:

\[ w_2 = \sqrt{-\frac{\lambda}{\pi i m(1/q_2)}}, R_2 = \frac{1}{Re(1/q_2)} \] \hspace{1cm} (3.2.12)

For the beam from undulator at beamline P23 it’s known that it has size \( w_u = 0.282 \ mm \) (horizontal) – on the exit of undulator and \( w_{60} \) – after 60 m of propagation (depends on energy), but radii of curvature and beam waist \( w_0 \) are unknown. They could be calculated from eq. (3.2.10):

\[ \begin{cases} w_u = w_0 \sqrt{1 + \left( \frac{x_0 \lambda}{\pi w_0} \right)^2} \\ w_{60} = w_0 \sqrt{1 + \left( \frac{(z_0 + \Delta z) \lambda}{\pi w_0} \right)^2} \end{cases} \] \hspace{1cm} (3.2.13)

here \( z_0 \) – distance from point when \( w = w_0 \) to exit of undulator, \( \Delta z = 60000 \ mm \) – distance from source to first transfocator. So, from (3.2.13):
\[ w_0 = \sqrt{\frac{c^2 w_a^2 - 2ab + \sqrt{a^2 + c^2}}{2(a^2 + c^2)}} \]

\[ a = \frac{\pi}{2}(w_a^2 - w_{b0}^2) \]

\[ b = \Delta z^2 \lambda^2 \]

\[ c = 2\Delta z \lambda \pi \]

\[ d = (2ab - c^2 w_a^2) - 4(a^2 + c^2)b^2 \]
4 Software implementation

Software is written in Python programming language with Python(x,y) development kit – it is a free scientific and engineering development software for numerical computations, data analysis and data visualization based on Python v.2.7.

Software for calculation parameters of CRL optic system has 3 modules:

1) Main module (“TS_matrix_optics_XX”) is responsible for:
   - Choosing and optimizing CRL transfocators in conformity with geometry of the setup and x-ray source properties.
   - Calculation ray transfer matrices for optical systems.
   - Calculation of beam size at any point of optical system.
   - Managing other modules and general calculation flow.
   This module is described in details in 4.1.

2) Module for calculation of photon flux transmitted through transfocators (“TS_transmission_gauss_module_XX”). The description is in part 4.2.

3) Service module (“TS_read_data”) which is used for reading miscellaneous data (initial beam sizes, optical constants, etc.) from hard disk. It has 3 functions:
   - size_calc – reads size of beam (FWHM) on 60 m from undulator for chosen energy of photons.
   - delta_calc – reads refraction index for chosen x-ray energy.
   - mu_calc – reads linear absorption coefficient for chosen energy (Energy) of photons.

Note: In modules functions/classes with names started from “_” are used only as an auxiliary ones for other modules/classes. Only “user-available” functions will be described below.

4.1 General calculation flow, optics optimization and geometry

The current version of software allows to calculate parameters of two transfocators (and their combinations) from given lens setup and, vice versa, to select best combination of lenses in transfocators to achieve desirable imaging conditions.

In software transfocators are represented as list objects in format:

```
[[N1, N2, ...], [R1, R2, ...], [d1, d2, ...], l]
```

here Ni – number of lenses one type, Ri – radius of curvature of parabola, di – distance between peeks of parabolic surfaces in lens, l – thickness of one lens (see part 3.1).

Global input parameters are:
- energy_min, energy_max, energy_step – range of energy for calculation: [energy_min, energy_max] with step energy_step.
– `dist_Src_TS1`, `dist_TS1_TS2`, `dist_TS2_Sample` – distances from undulator to first transfocator, between transficators, from second transfocator to sample respectively.

– `dist_TS1_image1` (`dist_TS2_image2`) – desirable distance from first (second) transfocator to image created by it.

– `Source_hor_0` (`Source_ver_0`) – beam size (FWHM) on the exit of the undulator.

– `R_set1` (`R_set2`) – list of radii of lenses that are allowed to use in first (second) transfocator.

– `lens_groups11` (`lens_groups21`) – groups of lenses of 1st radius that are allowed to use in 1st (2nd) transfocator.

– `lens_groups12` (`lens_groups22`) – groups of lenses of 2nd radius that are allowed to use in 1st (2nd) transfocator.

**Choosing the transfocator**

`build_TS_from_dist` – Makes a list of transficators from specified group of lenses with specified radii which create an image of object on appropriate distance from transfocator.

**Matrix optics**

`All_elements` (class) – the object of this class is a list of all elements in optical system. This list contains an index number of the element, information about type of element (free space or lens) and parameter of every element (length of space of focus of lens), it looks like:

<table>
<thead>
<tr>
<th>n</th>
<th>type</th>
<th>parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td><code>space</code></td>
<td>60000</td>
</tr>
<tr>
<td>1</td>
<td><code>lens</code></td>
<td>495000</td>
</tr>
<tr>
<td>2</td>
<td><code>space</code></td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td><code>lens</code></td>
<td>495000</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

`system_matrix` – makes a matrix of optical system from the list of elements (`'All_elements'` class object). It uses matrix formalism from part 3.2 (eq. 3.2.1 – 3.2.4).

`cardinal_points` – calculates distances to cardinal points of the optical system – see eq. 3.2.5 - 3.2.7

**Beam size calculation**

`size_calc_geometry` – calculates size of beam on the out of optical system using conventional geometrical optics laws:

\[
\frac{1}{f} = \frac{1}{a} + \frac{1}{b} = \frac{h_{out}}{h_{in}}
\]  

(4.1.1)

here \(a\) is distance from object to first principal plane, \(b\) – from second principal plane to image, \(h_{in}\) – size of object and \(h_{out}\) – size of image in the image plane. To know size of beam not only in image plane, approximate equation is used:

\[
h_{out}^* = h_{out} + |x_{out}|
\]  

(4.1.2)
where $x_{out}$ – coordinate of beam that entered the system at optical axis with angle $\theta/2$ ($\theta$ – beam divergency):

$$
\begin{pmatrix}
  x_{out} \\
  a_{out}
\end{pmatrix} =
\begin{pmatrix}
  A & B \\
  C & D
\end{pmatrix}
\begin{pmatrix}
  0 \\
  \theta/2
\end{pmatrix} 
$$

(4.1.3)

size_calc_wave_parameter – calculates beam size from transformation of complex beam parameter – see eq. 3.2.8 – 3.2.13.

### 4.2 Transmission and beam loss factor

Absorption of monochromatic beam in matter is described with Beer–Lambert law:

$$
I = I_0 \exp(-\mu x)
$$

(4.2.1)

where $\mu$ is a linear absorption coefficient, $x$ – thickness of material, $I_0$ and $I$ – initial intensity of x-rays and intensity after propagation through material.

For a CRL with $N$ parabolic lenses with radius of aperture $R_0$, radius of curvature of parabolas $R$ and distance $d$ between parabolas (fig. 3.1.2) beam loss factor is [3]:

$$
T = \frac{I}{I_0} = \exp(-\mu N d) \frac{1}{a_p} \left(1 - \exp(-a_p)\right)
$$

$$
a_p = \frac{\mu N R_0^2}{R}
$$

(4.2.2)

Unfortunately, this equation works only for beams with uniform distribution of intensity. For beam with Gaussian distribution (with standard deviations $\sigma_x$, $\sigma_y$ in horizontal and vertical directions) of intensity:

$$
I_0 = A \exp\left(-\frac{x^2}{2\sigma_x^2}\right) \exp\left(-\frac{y^2}{2\sigma_y^2}\right)
$$

(4.2.3)

beam loss factor is calculated analytically in quite complex way [1]. But it’s easy to calculate beam loss factor numerically: just use eq. 4.2.1 in every point of every lens and then divide sum of intensity after the CRL by sum of intensity before CRL.

There is only one user-available function in TS_transmission_gauss_module: calculate – it calculates the transmission numerically as described above. One important thing – it’s assumed that paraxial approximation for optical system is working (== size of beam is changed negligible during propagation through CRL).

### 4.3 Output
As a result, software creates a text file for every transfocator with a table of lens combinations for specified range of energies with calculated focus, beam loss factor, and size of beam. Example of such list – see figure 4.3.1. Legend for a table:

- **E(eV)** – energy of photons
- **R** – radii of curvature of lens parabola
- **N** – corresponding number of lenses
- **F_pos** – coordinate of focus (from undulator)
- **Im_pos** – coordinate of image (from undulator)
- **T** – transmitted amount of light
- **HorSize (VerSize)** – horizontal (vertical) FWHM of beam (at the entrance of the 2nd transfocator or on sample)

![Table of transfocators](data:image/png;base64,iVBORw0KGgoAAAANSUhEUgAAAIcAAAAPCAYAAABgYzhaAAAABGdBTUEAALGPC/xhBQAAAAB2FZpT/l0AAAABXRU5ErkJggg...)

*Figure 4.3.1 – Example of list of transfocators*
5 Application examples

The typical distances between optical components in P23 could be: undulator - transfocator 1 – 60 m, transfocator 1 - transfocator 2 – 26 m, transfocator 2 - sample – 1 m. This values will be used for examples in this chapter.

5.1 Single transfocator

The simplest optical system is one transfocator that focuses the beam onto the sample, so distance from transfocator to image will be

$$(\text{dist. transf.1 - transf.2}) + (\text{dist. transf.2 - sample}) = 27 \text{ m}$$

To calculate size of beam geometrical optics approach was used. From figures 5.1.1 – 5.1.2 it’s seen that it makes no sense to use lenses with 1.5 and 1.0 radii especially on higher energies because their number becomes too large and transmission decreases.

<table>
<thead>
<tr>
<th>Transfocator system #1</th>
<th>Image pos. = -27000.0 mm</th>
<th>Lens radii: [0.5, 0.3]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Groups of lenses: [2, 3, 5, 13] [2, 3, 5, 13]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Src - TS1 = -60000.0 mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TS1 - TS2 = 37000.0 mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TS2 - Sample = 0.0 mm</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

![Figure 5.1.1. List of transfocators made from 0.5 and 0.3 mm lenses](image-url)
5.2 Two transfocators (parallel beam)

Another important case – to make a parallel beam (telescope). It means that image plane of 1st transfocator should be matched with a focal plane of the second transfocator. Results for such transfocator system is in fig.5.2.1.
Figure 5.2.1. 1st transfocators for telescope

Figure 5.2.2. 2nd transfocators for telescope

5.3 Two transfocators (“aperture matching”)

“Aperture matching” means that first transfocator pre-focuses beam to aperture of the second one. The second transfocator should have a quite short focus distance in this case. This approach allows to achieve smallest spot on the sample. After tests of transfocators made from lenses with radii 1.5, 1.0, 0.5, 0.3, 0.1 mm, was concluded that transfocator with best transmission coefficient for whole range of energies could be built from 0.5, 0.3 mm (1st tr.) and 0.1 mm (2nd tr.) lenses (fig. 5.3.1-5.3.2).
Figure 5.3.1. 1st transfocator for aperture matching case

Figure 5.3.2. 2nd transfocator for aperture matching case
5.4 Selection of beam size calculation method

On figure 5.4.1 horizontal and vertical size of beam after the out of second transfocator (aperture matching case) are shown. Size was calculated by geometrical optics (4.1) and using wave parameter approach (3.2).

![Figure 5.4.1. Horizontal and vertical size of beam after the out of second transfocator](image)

Such large difference could be explained by fact that wave parameter approach is valid only for coherent beams, while the radiation after undulator has both coherent and incoherent fractions (fig. 5.4.2).

![Figure 5.4.2. Coherent fraction of x-rays from undulator](image)
Conclusion

A new software package was created, tested and used for beamline CRL optics design. Software is written in Python, has a modular structure. Typical scenarios of beamline CRL layout were tested: one transfocator, telescope, aperture matching. The modules developed in this work will become a part of beamline operation software at the Russian-German nanodiffraction beamline at PETRA.

Acknowledgement

I would like to thank Jana Raabe for her friendly support and cooperation during my stay at DESY.

References