# X-RAY POWDER DIFFRACTION BEAMLINE FOR IRANIAN LIGHT SOURCE FACILITY

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*Abstract*

X-ray Powder Diffraction beamline is one of the first priorities of Iranian Light Source Facility day-one-beamlines. This beamline will cover the research requirements of scientific community in the fields of physics, material science, chemistry, etc and also have benefits for industries. This paper shortly reports the ray tracing calculations for the optical design of this beamline. The results show that bending magnet source would satisfy the nowadays users requirements, although insertion device should also be considered for covering the requirements of the future users. In this paper the effects of the optical elements on the users' requirements have been discussed to obtain the appropriate design.

## INTRODUCTION

Iranian Light Source Facility (ILSF) project has been initiated since 2010 in order to design and construction of a third generation synchrotron facility for developing basic and engineering researches in Iran [1]. In parallel to the design and construction of the accelerator machine, a scientific division has been formed to reach the purpose of capacity building, organizing the users' community, design and construction of the ILSF beamlines. Seven day-one beamlines with its users' requirements has been specified by the users' community. X-ray Powder Diffraction (XPD) beamline is one of the most priorities in ILSF beamlines due to wide range of applications and big potential user community in Iran. ILSF Beam dynamic group has reported the design of the ILSF storage ring which gives us the electron beam parameters in the bending magnet (BM) and insertion devices [2]. All the parameters for BM and the electron beam inside the BM have been determined in this design; however the insertion devices have not been specified yet. So, in this study we have considered the BM source for pre-design stage of XPD beamline. However it is also helpful to consider an insertion device source for this beamline in the future studies and compare the results with the BM case.

## COMPUTATIONAL DETAILS

The radiated brilliance and photon flux of the BM source has been calculated by the SPECTRA code [3] and analytical formula for BM radiation [4]. The source parameters have been taken from ILSF beam dynamic calculations (see Table 2) [1]. The ray tracing calculations of the photon beam has been done by XOP and SHADOW codes [5]. The optical design parameters like optical distances and foot print have been optimized by fitting the results of calculation and users requirements. The optical properties of the optical elements such as reflectivity, absorbance, Bragg diffraction, rocking curve, aberration, etc have also been calculated to determine the optical elements specifications.

## BEAMLINE OVERVIEW

Main characteristic of ILSF XPD beamline including the users' requirements (four last lines) [1] are presented in Table 1. The spot size has been considered in the range of 0.1×0.1 to 10×1 $mm^2$ to cover more scientific cases.

Table 1: Characteristics of ILSF XPD Beamline

| Source | Bending Magnet (BM) |
|---|---|
| Optics | Collimating mirror, Si(111) DCM, focusing mirror |
| Photon energy range | 6-30 keV |
| Photon flux at sample | $10^{12}$ ph/s |
| Energy resolution (ΔE/E) | $10^{-4}$ |
| Spot size at sample (H×V) | 0.1×0.1- 10×1 $mm^2$ |

## SOURCE

Source of this beamline is BM with 1.42 T magnetic field strength. Important parameters of the BM source and the electron beam parameters are shown in Table 2.

Table 2: Important Parameters of BM Source, Electron and Photon Beam at Source Place of the XPD Beamline

| Parameter | Unit | Value |
|---|---|---|
| **ILSF storage ring energy** | GeV | 3 |
| Magnetic field | T | 1.42 |
| Critical energy | keV | 8.5 |
| Electron beam size (FWHM) | $\mu m^2$ | 109×60 |
| Electron beam divergence (FWHM) | $\mu rad^2$ | 206×3 |
| Photon beam size (FWHM) | $\mu m^2$ | 109×60 |
| Photon beam divergence (FWHM) | $\mu rad^2$ | 1500×284 |

### *Vertical Divergence*

The radiated photon beam divergence is mostly determined by the intrinsic divergence of the photon beam because of the lower divergence values of the electron beam. Intrinsic vertical divergence of photon beam is calculated approximately by $(560/\gamma)\times(\lambda/\lambda_c)^{0.43}$ as a function of energy, where $\gamma$ , $\lambda$ and $\lambda_c$ are the ratio of the energy to the rest mass of the electron, wavelength and critical wavelength of synchrotron radiation, respectively. The maximum value of vertical divergence calculated from this formula is 284 µrad (at 6 keV) inserted in table 2. Reducing of this value is very important for improving the energy resolution and vertical size of slits which will be discussed through this paper.

### *Photon Flux and Brilliance*

Photon flux and brilliance of ILSF BM source calculated by SPECTRA are shown in Fig. 1. The current of the beam is considered as I=400 mA.

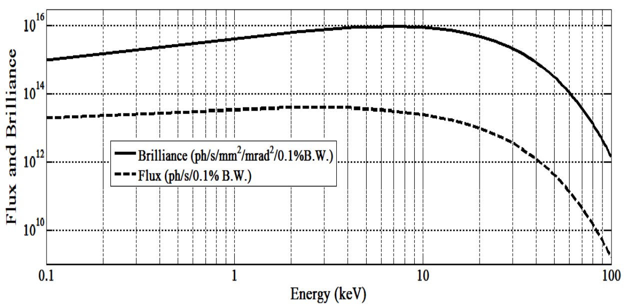


Figure 1: Photon flux and brilliance of ILSF BM source versus energy at I=400 mA and horizontal divergence of 1.5 mrad.

As it can be seen from Fig. 1, the flux and brilliance of BM in energy range of 6-30 keV are changing in the $3.5\times10^{12}$-$3.5\times10^{13}$ ph/s and 2.1-$9\times10^{15}$ ph/s/mm$^2$/mrad$^2$ in 0.1% band width (B.W.) ranges, respectively. Maximum power density radiation calculated from this BM is about 0.25 kW/mrad. Optical elements, especially before the monochromator, have to be cooled to load this heating.

## OPTICAL LAYOUT

Optical layout of the beamline is given in Fig. 2. This beamline consist of a cylindrical vertically collimating mirror (M1), Double Crystal Monochromator (DCM) with sagittaly focusing by second crystal, and a cylindrical vertically focusing mirror (M2). This layout is most common layout for XPD in different synchrotrons [6-8]. Total length of the beamline (source to sample) is considered to be 40 m.

### *Collimating Mirror*

First optical element is a cylindrical mirror that vertically collimates the beam. This mirror can be coated by Pt because of high reflectivity of this coating in the 6-30 keV range. By the way, as reflection calculation shows in Fig. 3 the incidence angle should be less than 2.5 mrad for reaching the high reflectivity in this range.

Ray-tracing calculation indicates that by changing the collimating mirror position in 8-22 m range from source, radius of the mirror has to be changed from 6.4 to 17.6 km to reach 6 µrad vertical convergence, and finally the horizontal foot print of photon beam on M1 changes from 90 to 250 cm at 2.5 mrad incident angle. So, the appropriate position of the M1 could be 15 m to have reasonable mirror size and less challenge in the heatload. In this distance the M1 bending radius is 10 km and the foot print of the photon beam on M1 is 120×2 cm$^2$. This element alters 284 µrad vertical divergence to 6 µrad convergence (less than the Darwin width of Si(111)) in these conditions to improve the energy resolution.

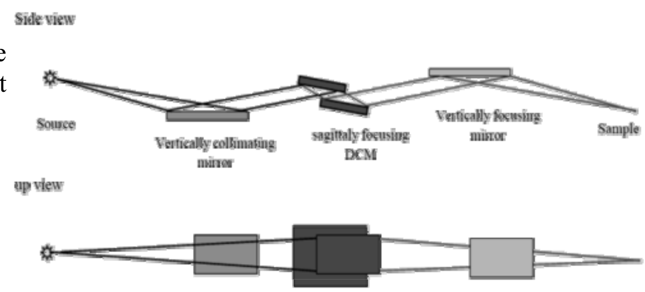


Figure 2: Optical layout of XPD beamline consist of a collimating mirror, sagittaly focusing DCM and a vertically focusing mirror.

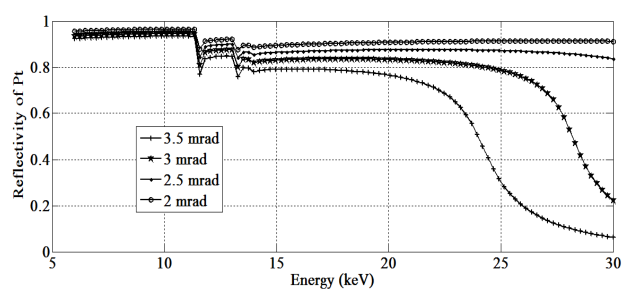


Figure 3: reflectivity of Pt at different incidence angles in the desired photon energy range: 6-30 keV.

### *Double Crystal Monochromator*

Monochromator of XPD beamline is double crystal Si(111) that its second crystal could be bent sagittaly to focus the beam horizontally. The place of DCM is at middle of the beamline (20 m) to reach low aberration at sample position. Footprint on the first crystals is about 2×3 cm$^2$. Energy resolution of the perfect flat crystal is calculated by equation 1, however for the bending crystal, the bending radius should be considered. ΔE/E has been calculated for flat crystals to be $1.4\times10^{-4}$ for 6-30 keV from ray tracing calculations in comparable to the result from equation 1.

$$\frac{\Delta E}{E} = \sqrt{\Delta\theta_{\text{int}}{}^{2} + \Sigma_z'^{\,2}}\,\cot\theta \qquad (1)$$

where, ΔE/E: relative energy resolution, $\Delta\theta_{int}$: Darwin width, $\sum'_z$: beam divergence, θ: incidence angle.


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### *Focusing Mirror*

M2 is a bendable cylindrical mirror with Pt coating to focus the photon beam vertically at the sample position. Ray-tracing calculation indicates that by inserting the M2 distance as 25 m from the source and its bending radius as 10 km in 8 keV, the aberration of photon beam at sample position is decreased.

Figures 4 and 5 show the results of the changes of the vertical and horizontal spot size of the photon beam at the sample position versus the radius of M2 and DCM respectively. These data has been derived from the FWHM of the photon distribution calculations which a typical one is presented in Fig. 6. These values are dependent to the photon energy and so considered in 8 keV.

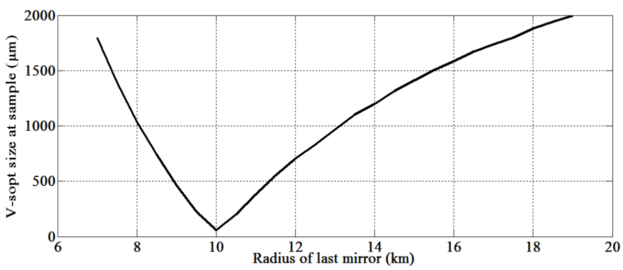


Figure 4: Variation of vertical (V) spot size at sample position versus last mirror radius.

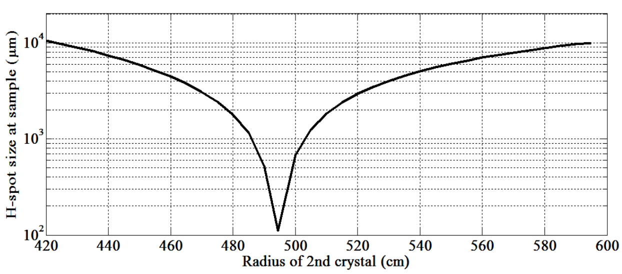


Figure 5: Variation of horizontal (H) spot size at sample position versus 2nd crystal radius.

Figure 4 shows that the vertical spot size at sample position is changed from 100 μm to 1 mm by changing M2 radius from 8 to 10 km or 10 to 13 km. From Fig. 5, it is seen that the horizontal spot size changes from 100 μm to 10 mm by changing of radius of the crystal from about 420 to 490 or 490 to 590 cm. So, there are two options for each case, however due to the easier mechanics and higher controls larger radius is suggested.

## FLUX AT SAMPLE

The reflectivity of the mirrors and the energy band pass of the monochromator specify amount of the flux at sample. Figure 7 shows the photon flux after the optical elements: Be window, M1 and M2, versus photon energy. Thickness of Be window is 200 μm in this calculation. Calculations show that ideally (without considering the roughness of the mirrors, etc) about 80 percent of the radiated photon in the bandwidth of monochormator is reached to the sample.

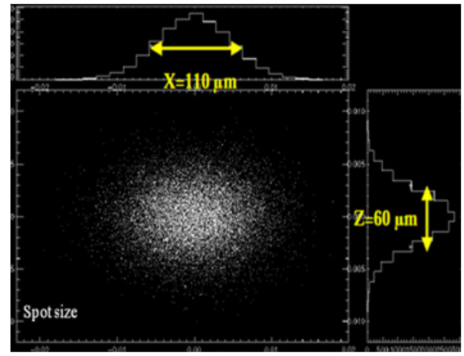


Figure 6: Distribution of photons at sample position (8 keV). The FWHM of the spot size is indicated in the figure.

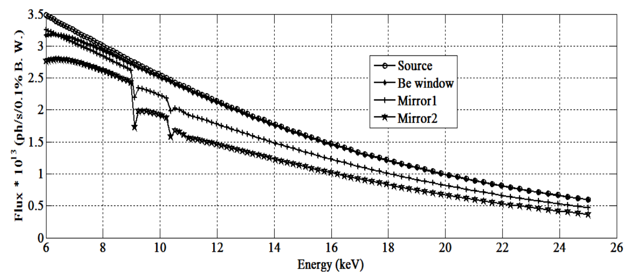


Figure 7: Photon flux after Be window, M1 and M2 mirrors in 6-25 energy range.

## CONCLUSION

Ray-tracing calculation was used to design of XPD beamline of ILSF. It has been concluded that by standard layout and optimization of the design parameters the users' requirements could be reached. The spot size and photon flux at the sample position are reasonable and can be adjusted by changing the M1 and DCM radiuses.

## REFERENCES

[1] ILSF CDR: http://ilsf.ipm.ac.ir/Publications/ILSF-CDR.pdf
[2] H. Ghasem, F. Saeidi, E. Ahmadi, "Lattice Candidates For The Ilsf Storage Ring", Proceedings of IPAC2011, San Sebastián, Spain
[3] T. Tanaka and H. Kitamura, J. Synchrotron radiation 8, 1221 (2001).
[4] H. Wiedemann, "Synchrotron Radiation", Springer, 2002
[5] http://www.esrf.eu/usersandscience/experiments/TBSscisoft/xop2.3
[6] Kia S. Wallwork et al, "The High Resolution Powder Diffraction Beamline for the Australian Synchrotron", AIP Conf. Proc. 879, 879 (2007)
[7] B.D. Patterson et al, "The Materials Science Beamline at the Swiss Light Source", Nuclear Instruments and Methods in Physics Research A 540 (2005) 42–67
[8] A.N. Fitch, "The High Resolution Powder Diffraction Beamline at ESRF", J. Res. Natl. Inst. Stand. Technol. 109, 133-142 (2004)