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NSLS-II Biomedical Beamlines for Macromolecular Crystallography, FMX and AMX, and for X-ray Scattering, LIX: Current Developments

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Abstract. We present the current status of development of the two macromolecular crystallography (MX) beamlines, FMX and AMX, and the X-ray scattering beamline LIX, at the National Synchrotron Light Source-II (NSLS-II) [1]. Together, FMX and AMX will cover a broad range of use cases from serial crystallography on micron sized crystals, to very large unit cell complexes, to rapid sample screening, e.g. for the always-hard-to-grow membrane proteins and for ligand binding studies. The LIX beamline will support a variety of X-ray scattering measurements for studies on proteins in solution, lipid membranes and biological tissues. We have performed Synchrotron Radiation Workshop (SRW) [2] and Shadow[3] simulations to help select optimal methods to modify the size of the beam easily and smoothly at both FMX and AMX. The very low emittance of the NSLS-II storage ring and the resulting low divergence of the X-ray beam, as well as the long optical path lengths in the photon delivery systems lead to stringent requirements e.g. for vibrational stability and mirror quality. We discuss beamline design considerations addressing these challenges, such as combining mirror optics with compound refractive lenses (CRLs).

1. Introduction

Funded by the National Institutes of Health and the Department of Energy, the suite of Advanced Beamlines for Biological Investigations with X-rays (ABBIX) is scheduled to begin open user operation by 2016. The pair of MX beamlines is located at two identical canted undulators (IVU21) in sector 17-ID. The beamlines’ specializations are complementary. The FMX beamline, for Frontier Microfocusing Macromolecular Crystallography, will deliver a high photon flux of $10^{13}$ ph/s at a wavelength of 1 Å into a spot of 1 μm width. It will cover a broad energy range of 5 – 30 keV, corresponding to wavelengths from 0.4 – 2.5 Å. Beam sizes up to 50 μm will be available. The AMX beamline, for Highly Automated Macromolecular Crystallography, will be optimized for high throughput applications, with beam sizes from 4 – 100 μm and an energy range of 5 – 18 keV (0.7 – 2.5 Å). The LIX beamline, for High Brightness X-ray Scattering for Life Sciences, will be accommodated in the neighboring sector 16-ID. Equipped with a single long undulator (IVU23), it will produce beams down to a size of ~1 μm via a two stage demagnification scheme, involving

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mirrors and CRLs, and up to several hundred microns in size. It will have a broad energy range of 2.1 – 18 keV (0.7 – 5.9 Å) and be capable of simultaneously collecting data on three detectors.

2. Beam expansion
A variable beamsize is required to match the beam size to varying crystal sizes[4]. Additionally, for diffraction based crystal alignment schemes, rapid beam size increases to cover a large rastering area and locate crystals need to be interleaved with reliable refocusing for data acquisition on micron sized crystals. The secondary focusing stage of the FMX beamline will combine CRLs and Kirkpatrick-Baez (KB) focusing mirrors. For data acquisition, the curvature of the KB mirrors will be adjusted to move the focus downstream and match the beam size to the crystal size at the sample position. For rastering, by inserting CRLs upstream of the KB mirrors, the focus is moved upstream of the sample and thereby rapidly expands the beam size. By retracting the CRLs, the users can return within seconds to the optimized micro beam for crystallographic data acquisition.

In either focusing scheme, the figure errors of the mirrors will dominate both the minimally achievable beam size and the intensity variations on expanded beams. As beam distortions due to CRL inhomogeneities will be significantly smaller than distortions due mirror figure errors[5], all calculations have been performed assuming ideal lens shapes.

3. X-ray optics simulations
To derive specifications requirements for the mirror figure errors and avoid costly over-specifications, simulations were carried out both with the ray tracing package Shadow[3], and with the wavefront propagation package SRW[2]. To obtain a realistic estimate for the influence of mirror figure errors, both simulations were carried out using a measured (size) mirror file of the MISTRAL beamline at the ALBA Synchrotron (courtesy Josep Nicolas, ALBA, Spain). Its central 500 mm length section has a residual slope error (rms) \( \delta = 0.1 \) μrad and a height error (rms) of 7 nm (P-V = 21 nm). With this, the slope error limited vertical beamsize (fwhm) at an image distance of \( q = 1.1 \) m can be estimated to 2×2.35\( \delta q \) = 0.5 μm in good agreement with the simulated focus (figure 1, left). In SRW, the elliptical shapes of the KB mirrors were implemented using a grazing-incidence “thick optical element” propagator based on local ray-tracing. The KB surface height error was simulated by corresponding phase shifts (“masks”) in the transverse plane at the mirror location.

Due to the very small vertical emittance of the NSLS-II electron beam, the largest effect from the mirror figure errors are expected in the vertical direction. In the SRW-simulated beam profiles with and without mirror figure errors, significant modulations up to 20 % of the unperturbed profile can be observed, both for the focused beam spot at the sample position (figure 1, left) as well as for the beam defocused by insertion of CRLs upstream of the vertical KB mirror (figure 1, right).

Figure 1. X-ray intensity distribution in vertical median plane calculated with SRW[2] at the sample position of the FMX beamline, for cases of best focusing (left) and defocusing using CRLs (right).
To obtain a quantitative estimate of the transverse coherence, a “virtual Young’s slit experiment” was simulated in SRW (figure 2) and the fringe visibility $F = (I_{\text{max}} - I_{\text{min}}) / (I_{\text{max}} + I_{\text{min}})$ evaluated. The slit separation at half height is 270 µm for the vertical KB- and 22 µm for the horizontal KB-slits, providing a good estimate for the transverse coherence length at the FMX vertical KB mirror position.

Based on the van Cittert – Zernike theorem, for an extended incoherent source with a Gaussian density distribution in the transverse plane with different points emitting uncorrelated spherical waves, the fringe visibility after a Young’s slit pair can be calculated analytically:

$$F = \exp\left(-2\left(\sigma h / \lambda R\right)^2\right),$$

where $h$ is the slit separation, $\sigma$ is the RMS source size, $\lambda$ is the wavelength, and $R$ is the distance to the source (figure 3). For the vertical slit separation plot, the values from the wavefront propagation agree very well with the calculation. For the horizontal case, the agreement is good with the exception of the higher fringe visibility in the SRW simulation at a separation of 100 µm, likely due to partial coherence at the secondary source, which in the analytical estimation is assumed to be incoherent.

**Figure 2.** Intensity distributions in the vertical median plane 20 m downstream of a Young’s slit pair at the position of the FMX vertical focusing KB mirror as a function of slit separation of 2 µm wide vertical slits.

These simulations provide clear evidence that even at the most critical mirror position the focusing is not dominated by coherence effects. However, with the vertical transverse coherence length being a significant fraction of approximately 1/6 of the total beam height, for the vertical KB mirrors for the AMX and FMX beamlines we used the Marechal criterion of the maximum tolerable wavefront error $< \lambda/14$ rms to specify a maximum rms height error. For an incidence angle $\theta = 2.5$ mrad at a wavelength of 1 Å, this limits the height error (rms) to $< 1.5$ nm.

4. **Stability requirements of the double crystal monochromators (DCM)**

The DCM with its central position in the photon delivery system is crucial to the beam stability. As both crystals have to be cooled with liquid nitrogen, they are subject to vibrational excitations from the cooling systems. To determine the maximally acceptable angular vibration amplitude for a DCM crystal, we assume a maximal vertical deviation of 10 % of the focal spot size of 500 nm at FMX. With a demagnification of 60, a deviation of 3 µm of the source position leads to this focus spot deviation. An angular deviation of a crystal to the downstream optics is indistinguishable from a source movement. A $2\theta$ angular deviation corresponding to a 3 µm vertical source deviation is 75 nrad. For a single FMX DCM crystal and uncorrelated vibrations, the maximum deviation is 27 nrad. For AMX, an analogous estimate for the maximum $2\theta$ angular deviation is 200 nrad.

The extreme angular stability requirement for FMX is a strong indication for a DCM geometry with a vertical axis, as this facilitates construction of a less vibration-sensitive design[6]. For AMX,
both the less stringent angular stability requirement and the close proximity of the FMX white beam at the position of the AMX DCM indicate a design with a horizontal rotation axis.

5. LiX beamline layout

The optical layout of the LiX beamline has been revised since our last report[1]. The LiX monochromator will have two sets of interchangeable Si(111) crystals: a double crystal set to maintain a constant exiting beam height throughout the full energy range, and a channel-cut crystal for high stability used above 10keV. The first optical element is now a flat white beam mirror that deflects upward, which reduces the incident power onto the monochromator crystal, especially at low X-ray energies (~46 % at 3.6 keV). The vertical focusing mirror of the KB pair then deflects the beam downward by the same angle, so that the x-ray beam falls in the horizontal plane in the endstation.

The secondary source aperture is integrated into the same vacuum enclosure with several beam diagnostic components. The CRL transfocator is mounted on a long travel linear stage to provide variable demagnification and to compensate for the X-ray energy-dependence of the CRL focal length.

Conclusion

Critical details of the conceptual layout[1] for the FMX and AMX beamlines have been investigated. The optical and stability requirements due to the micron sized X-ray beam foci and the extremely low emittance of the NSLS-II electron beam were shown to be achievable with state of the art technology.

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