Design of the X-ray Nanoprobe Beamline at the Taiwan Photon Source

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Abstract. The X-ray Nanoprobe (XNP) Beamline Project has been granted as one of the first seven beamlines at the Taiwan Photon Source (TPS). The XNP beamline and the associated instruments are designed to utilize the highly brilliant TPS light source for resolving the atomic, chemical and electronic structures of semiconductor-based devices with tens nm spatial resolution in tomographic and nondestructive manners. The beamline optics is deliberated to deliver focal spot around 40 nm with photon flux in the level of $10^{10}$ photons/sec. The stability of the focal position will be highly improved by operating the double crystal monochromator (DCM) in horizontally diffracting geometry, with minor sacrifice in energy resolution. The relative movement between sample and focusing optics is controlled by ultra-precise linear translational/flexure stages and monitored by laser interferometers. The end stations will provide conventional X-ray probes including, X-ray fluorescence (XRF), X-ray absorption fine structures (XAFS), X-ray excited optical luminescence (XEOL), and the emerging techniques, such as the Bragg-ptychography (BP) to overcome the spatial resolution set by the focusing optics. A novel scanning mechanism incorporating surface diffraction and BP for mapping the 3D interfacial strains is under development. The XNP beamline and associated instruments are expected to take the first synchrotron light by the end of 2015.

1. Introduction

A modern synchrotron-based X-ray Nanoprobe (XNP) beamline is expected to provide a wide variety of probing capabilities with tens-nm spatial resolution, in spectroscopy, microscopy and diffraction [1]. In order to fulfill the wide requirements from various kinds of X-ray techniques, several design criteria are taken for a modern XNP beamline: (1) minimizing the number of beamline optical elements to preserve the source coherence; (2) nano-focusing optics with diffraction-limit spot; (3) high throughput optics; (4) achromatic optics is preferred; (5) large working distance; (6) minimizing the mechanical and ground instability.

The XNP at the TPS is designed to provide conventional X-ray probes in the energy range 4-15 keV as well as the emerging techniques such as Bragg ptychography (BP) employing coherent X-rays. The beamline will consist of one horizontal focusing mirror (HFM), a horizontally diffracting monochromator before the nano-focusing optics. It will operate without X-ray windows, maintaining vacuum environment from the upstream beamline optics to the samples. The nested Montel mirrors [2] are chosen as the nano-focusing optics for the reasons of easy alignment, achromatic in a wide energy range and high photon throughput. The ultimate focal spot is expected around 40 nm at the sample, with photon flux in the level of $10^{10}$ - $10^{11}$ photons/sec with energy resolution $2\times10^4$. 

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2. Photon source
The beamline utilizes the light source generated from an in vacuum undulator IU22 with nominal period length 22 mm. The characteristic parameters of IU22 are tabulated in Table 1. The IU22 is positioned at the center of the 7m straight section of TPS. With the minimum gap of 5 mm, the IU22 is able to emit X-rays in the energy range 3.52 – 20 keV by continuously opening the undulator gap and switching among the harmonic number 3 – 15. The spectra of IU22 in term of brilliance and flux are calculated by SPECTRA and shown in Figure 1. The horizontal and vertical photon source sizes are calculated to be 282 \( \mu \text{m} \) and 14.8 – 12.5 \( \mu \text{m} \) (in full-width at half-maximum, FWHM), respectively, and the horizontal and vertical source divergences 48.2 – 45.1 \( \mu \text{rad} \) and 27.5 – 21.9 \( \mu \text{rad} \) (FWHM), respectively.

Table 1. IU22 Source Parameters at TPS

| Parameter                  | IU22               |
|----------------------------|--------------------|
| Photon energy (harmonic number 3 - 15) | 3.52 –20 keV        |
| Period length, \( \lambda \)          | 22 mm              |
| Number of period, \( N_{\text{period}} \) | 140                |
| Peak field                  | 1.05 T             |
| Deflection parameter, \( K_{y_{\text{max}}} \) | 2.15               |
| Total magnetic length       | 3.1 m              |
| Minimum magnet gap\( ^a \)     | 5 mm               |
| Total power @ 500 mA        | 9.7 kW             |
| Power density @ 500 mA      | 65 kW/mrad\( ^2 \) |

Figure 1. The brilliance (left) and the flux (right) emitted by a 3m-IU22 at ring current 500 mA.

3. Beamline design
The beamline, referring to Figure 2, is designed to deliver the maximum photon flux with the smallest reachable focal spot at the sample. A two-stage horizontal focusing strategy is taken. Starting from upstream, the first beamline optics is a water-cooled 700 mm-long horizontal focusing mirror (HFM) located at \( z = 24 \) m. With magnification 1:3, the HFM images the source downstream at \( z = 32 \) m where a secondary source is defined by a water-cooled beam-defining aperture (slits2). The Si-made HFM serves to suppress the high harmonic and heat load. The surface of the HFM is half-coated with Rh and the rest half uncoated. With 4 mrad incidence, the HFM reflects X-ray up to 16.9 keV. The
HFM deflects the beam horizontally to provide an offset of 360 mm at the sample position (z = 69 m) sufficient for safety requirement in avoiding directly seeing the source. The nano-focusing optics is a pair of nested Montel Rh-coated mirrors located at z = 69 m. With mirror length of 150 mm and an edge-clear working distance of 20 mm, the resultant demagnification ratio upon combining the HFM and the nested Montel mirrors is calculated to be 1/726 and 1/389 in vertical and horizontal direction, respectively. By assuming a 7 μm opening of beam-defining aperture, one can directly estimate the most optimistic focal spot at the sample position to be around 20 nm (FWHM) in both directions. The image burring caused by the diffraction-limit and the slope error of the nest mirrors will be discussed in next section.

The double crystal monochromator (DCM) with two Si(111) crystals is located at z = 66 m. The location of DCM is a trade-off decision balanced between the power density impinging on the DCM and the angular stability of the first with regard to the second crystal. Two strategies are taken to ensure the mechanical stability while scanning the DCM energy at fixed exit condition: (1) To count on the cause of gravity, the Si crystals are placed in horizontally diffracting geometry in which the rotational axes of the crystal are perpendicular to the ground surface; (2) An 8 mm gap between the two Si crystals is adapted to further reduce one translational stage alone z-direction. The total heat-load and power density impinging on the DCM can be much reduced with helps of front-end aperture and beamline slits. By locating DCM at Z= 66 m, the normal total heat-load and power density are estimated to be 0.2 W and 0.62 W/mm², respectively. For comparison, the power density on DCM is 68 times higher when the DCM is located at z = 33 m than that at 66 m. Despite that a water-cooling strategy seems feasible under such power density, the liquid nitrogen-cooling strategy is preferable at this stage of design.

The energy resolution of DCM is a resultant quantity determined by the Darwin width of Si (111) crystals, the angular size of the secondary source subtended at the monochromator and the angular acceptance practically set by the downstream nano-optics [3]. In the present design, the source-subtending angle is 0.2 μrad (FWHM). The horizontal angular acceptance of the DCM is calculated to be 16 μrad (FWHM), set by the location (z = 69 m), the length (150 mm) and the incident angle (4 mrad) of the nested Montel mirrors. The resultant energy resolution, despite not as good as intrinsic Darwin width of Si(111) (~1.4×10⁻⁴), is calculated less than 2×10⁻⁴ in 4 – 20 keV.

![Figure 2. Optical Layout of the X-ray Nanoprobe beamline at TPS.](image)

4. Expected Performance
The beamline performance is simulated by ray tracing program SHADOW. The final focal size is a convolving result of the geometric demagnification ratio, the slope error of mirrors and the effect of diffraction limit. The diffraction-limit spot size ε is estimated by ε ~ 0.88 λq/D [4]; where λ is the wavelength, q the image distance (95 mm), and D (0.6 mm) the projection aperture of nano-focusing optics.
mirrors. Fig 3a shows the simulated focal spot sizes at sample by setting a 7 μm horizontal opening of slits2, with three various slope errors of nested mirrors, 0 μrad (square), 0.05 μrad (triangle) and 0.1 μrad (circle), with the contributions from geometric demagnification (solid line) and diffraction-limit (dash line). The degree of coherence inside the focal spot can be approximately estimated by rationing the fractional area of the diffraction-limit spot occupied. In the case of nested mirrors with slope error of 0.05 μrad, the coherent fraction is 69% and 13% at energy 4 keV and 15 keV, respectively, resulting a coherent flux $10^{11} - 10^9$ photons/sec in the energy range 4 – 15 keV.

The simulated flux at the sample is shown in Fig 3b, with three alternative nano-focusing optics, namely, the nested Montel mirrors (Montel, circle), the conventional KB mirrors (KB, triangle) and the Fresnel zone plates (ZP, square). While a two-stage focusing is taken for the cases of Montel and ZP, the KB directly images the source at the sample. A horizontally diffracting DCM is employed. The edge-clear working distance for the three cases is kept 20 mm, and the diffraction efficiency of ZP is assumed 10%. The ultimate focal spot sizes are assumed same as the case of the Montel with slope error 0.05 μrad. The mirror length is 150 mm for Montel and 40 mm (H) × 100 mm (V) for KB. The incident angle for the mirrors is kept 4 mrad. The diameters of zone plates vary from 820 – 230 μm in energy range 4 – 15 keV. The higher flux throughput in the cases of Montel and KB than that of ZP is a direct result of optical efficiency of the nano-optics used. Advantaging by the geometric arrangement, the acceptant aperture for Montel is 0.6 mm (H) × 0.6 mm (V) over that of KB 0.16 mm (H) × 0.4 mm (V). However, the up-to-date optical efficiency of Montel is much lower than 70%, and the slope error of Montel mirrors is yet not reaching 0.05 μrad as expected in the simulation [2].

![Figure 3](image-url)

*Figure 3.* (a): Simulated focal spot sizes at sample with various slope errors of nested Montel mirrors 0.00 μrad (square), 0.05 μrad (triangle) and 0.10 μrad (circle), with the contributions from geometric demagnification (solid line) and diffraction-limit (dash line). (b): Comparison of the expected flux delivered at the sample with three alternative nano-focusing optics, the nested Montel mirrors (circle), the conventional K-B mirror (triangle) and the Fresnel zone-plate (square), with the flux spectra from IU22 (solid line).

5. References

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