CARNAÚBA: The Coherent X-Ray Nanoprobe Beamline for the Brazilian Synchrotron SIRIUS/LNLS

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Abstract. The CARNAÚBA beamline is the tender-to-hard X-ray (2 – 15 keV) scanning nanoprobe beamline planned for the 4th generation storage ring SIRIUS at the LNLS. CARNAÚBA uses an undulator source with vertical linear polarization in a low-beta straight section and grazing incidence-focusing mirrors to create a nanoprobe at 143 m from the source. The beamline optic is based on KB mirrors and provides high brilliance at an achromatic focal spot down to the diffraction limit diameter of ~30 nm with a working distance of ~6 cm. These characteristics are crucial for studying nanometric samples in experiments involving complex stages and environments. The CARNAÚBA beamline aims to perform raster scans using x-ray fluorescence, x-ray absorption spectroscopy, x-ray diffraction and coherent x-ray imaging techniques. Computed tomography will extend these methods to three dimensions.

1. Introduction

The Coherent X-Ray Nanoprobe Beamline (CARNAÚBA) is the tender-to-hard X-ray scanning nanoprobe beamline planned for the SIRIUS storage ring at the LNLS (Laboratório Nacional de Luz Síncrotron), Campinas, Brazil. The CARNAÚBA project aims to deliver to the scientific community a state-of-the-art nanoprobe based on a Kirkpatrick-Baez (KB) achromatic optic thus allowing for spectroscopic, resonant and imaging x-ray techniques. In order to face complex sample environments, the main goal is not to get record small spots but to have a nanoprobe with a stable beam and a comfortable working distance.

CARNAÚBA will deliver the smallest nanoprobe among the first phase SIRIUS beamlines. The beamline fully exploits the high brilliance and coherence characteristics of the X-ray beam delivered by the undulator source both for diffraction-limit focusing and contrast formation. It offers not only X-ray fluorescence (XRF) and X-ray absorption (XANES) spectroscopy, but also the most advanced multimodal coherent imaging techniques. CARNAÚBA is a unique research tool for a wide interdisciplinary user community working in the fields of agriculture, life-, earth-, environmental-, and materials science [1]. The beamline starts to be assembled in 2018. Many ideas and prototypes have been developed. Among them, a permanent magnet undulator with a few periods has been assembled (section 2) and a cryo-cooled four bounces x-ray monochromator has been designed (section 3). The assembling and commissioning phase will take place in 2019, when the first users will be welcome. In this paper we present CARNAÚBA’s design characteristics and expected performance.
2. The undulator source

The SIRIUS storage ring [2] has been designed to have a natural horizontal emittance of \( \epsilon_x = 245 \text{ pm rad} \) and a vertical emittance (coupling 1%) of \( \epsilon_y = 2.4 \text{ pm rad} \), without considering further reducing of the emittance by the insertion of undulators. The projected \( \beta \) values in the middle of the low-beta straight sections are \( \beta_x = 1.4 \text{ m} \) and \( \beta_y = 1.7 \text{ m} \), in the horizontal and vertical directions, respectively. The similar values of \( \beta \) have been chosen to reduce as much as possible both vertical and horizontal beam-stay-clear values to \( \approx 4.5 \text{ mm and } \approx 8 \text{ mm} \), respectively, as well as to optimize the photon flux emittance for an undulator of \( \approx 2.0 \text{ m} \). Such a singular condition for the \( \beta \) values allows using an undulator source with vertical linear polarization.

Linearly polarized light will be used for scattering, diffraction and absorption spectroscopy at CARNAÚBA. With linear polarization in the vertical, the scattering plane of the Si(111) crystal monochromator can be in the horizontal - to preserve a good vertical stability - without harming the flux close to the Brewster angle in the tender X-ray range.

The adopted solution for the CARNAÚBA insertion device has been a modified Delta undulator. The essential difference in the Delta design compared to the conventional one is that there is no gap variation: the field, or the K value, varies by changing the phase, i.e., by sliding one set of magnets along the beam related to the other [3]. Our modified Delta design has four sets of permanent magnets that can slide independently to provide a variable orientation magnetic field. A short prototype has been assembled and measured. Refined parameters for the final prototype will be available soon.

![Figure 1](Image)  

**Figure 1.** Left: Brilliance of the CARNAÚBA undulator with \( K_{\text{max}}=2.3 \) and 100 poles of 20 mm. Right: flux at the focal spot, within 0.01% bw and collecting a divergence of about 6x10 \( \mu \text{rad}^2 \) in the horizontal and vertical, respectively. The machine current is 350 mA. Vertical lines represent some light element K-edges.

To avoid gaps between the first and third harmonic of the undulator, a \( K_{\text{max}} \) of 2.05 or higher is required. Taking the beam-stay-clear values into consideration, a two-meter long undulator with 20 mm period and \( K_{\text{max}} \) of 2.3 is a possible configuration. The brilliance, as well as the total flux at the focus after the optics, of such undulator is presented in Figure 1. The undulator matches well the main applications of the CARNAÚBA beamline delivering energies from 2 keV up to 15 keV with very high brilliance. The vertical dashed lines represent the energy positions of some light elements K-edges (P, S, Cl, K, Ca, Ti, Cr), covered by the 1st and 3rd harmonics of the undulator. The total flux, taking into account the optics described in the next section, i.e., a bandwidth of the four crystal setup (\( \approx 0.01\% \text{bw} \)) with the machine running at 350 mA and a KB system collecting a divergence of 6x10 \( \mu \text{rad}^2 \), overpasses \( 10^{12} \) photons/sec at the focal spot. We should point out that the collected divergence selects the beam coherent fraction, meaning that the total flux corresponds to the fully coherent flux.

3. The optics

Source characteristics in 4th generation storage rings are normally limited by diffraction in the vertical (typical FWHM sizes of 10 \( \mu \text{m} \)) while still limited by emittance in the horizontal (about 50 \( \mu \text{m} \) at the SIRIUS undulator). With the available distance from the source at CARNAÚBA, 143 m, focusing to
smaller than 20 nm can be done in one step in the vertical by a mirror $M_V$ with a demagnification of about 500, leaving a working distance of about 30 cm. In the horizontal, this is not possible, and demagnification has to be done in two steps by using a secondary source aperture (SSA), which can then be slit down conveniently. With this choice, the horizontal mirror $M_H$ requires a larger demagnification than the vertical and has to be placed downstream in the sequential mounting in a KB system.

We used simple analytical expressions for geometrical optics beyond the thin lens approximation and a correction to account for the diffraction limit [4] to design and optimize the CARNAÚBA optical layout (Fig. 2). After white beam slits (WBS) defining a 50x50 $\mu$m$^2$ divergence, the mirror $M_1$ (at 27 m) creates a secondary source SSA (at 54 m) in the horizontal in a 1:1 configuration. The bremsstrahlung radiation shield (BRS) (at 30 m) stops the bremsstrahlung cascade 3 m after the $M_1$ mirror. The mirror $M_2$ (at 56 m) bounces the beam back, parallel to the original propagation. Both mirrors are used for harmonic rejection and may eventually be used to steer the beam at the SSA and at the experimental station, respectively. The harmonic rejection scheme of the primary optics, with the mirrors working at fixed grazing incidence of 5 mrad, employs three stripes, Rh, bare Si and Ni that can be selected by a vertical translation. A horizontal deflecting 4-bounces crystal monochromator (4CM) (at 136 m) close to the experimental station, select the photon energy with $E/\Delta E \approx 10000$. A prototype has been designed and will be assembled and tested in 2017. Pink beam mode may be used by sliding laterally the 4CM by a few mm. The nanoprobe station (at 143 m) holds the KB mirror system (with $M_V$ at 142.64 m and $M_H$ at 142.88 m), sample holder environment and detectors.

Figure 2. Layout of the CARNAÚBA beamline at the Sirius storage ring.

Considering, as a first approximation, ideal elliptical mirrors in the strong focusing approximation, the focus size is given by a convolution of the diffraction limit and the demagnified source. Trading between geometric demagnification and diffraction limit at the same time as the flux lead us to the optimized layout shown in Figure 2. The vertical and horizontal focus can be made very similar in size and divergence by adjusting the beam fraction collected at the SSA slit. This is shown in Figure 3 where the SSA aperture is set to 20 $\mu$m. One may note that for energies above 6 keV they are similar and kept below 50 nm. This is essentially due to the large numerical aperture of the KB mirror system ($\sim 5$ mrad) working at a maximum incidence angle of 5.6 mrad. The drawback of such a large numerical aperture is a limiting energy of about 15 keV due to the mirror cut-off. In the lowest energy side, below 6 keV, the focal spot increases, clearly limited by diffraction. In this range, the SSA aperture can be increased to gain more flux without enlarging the focus spot. For instance, using a 50 $\mu$m aperture, the flux density should increase by a factor 2 or more.
After the analytical ray tracing optimization, a hybrid ray tracing code was used to fully take into account all optical elements, including errors in the mirrors and the wave character of the propagation. Both calculations agree very well to each other, giving similar results in terms of flux of photons, divergences and nanoprobe sizes [4]. From these calculations, the primary optic, M₁ and M₂ mirrors, has to have slope figure errors smaller than 250 nrad. The thermal bump in the first mirror is negligible and does not affect the image at the SSA aperture. As far as the KB mirrors are concerned, the specifications are more stringent, in particular for the higher energies above 12 keV. The mirrors have specifications with slope figure errors of 50 nrad and, in addition, special care has to be taken with the spatial frequency domain that may cause some blurring at focus. The beam size at lower energies is almost diffraction limited and these errors showed to be negligible.

![Figure 3](image1.png)

**Figure 3.** Left: Energy dependence of the vertical and horizontal focus size. Right: Flux density at the focus, within 0.01% bw, collecting a divergence of about 6x10⁻⁵ μrad² in the horizontal and vertical, respectively, and with SSA aperture of 20 μm, with 350 mA in the machine. Vertical lines represent some light element K-edges.

4. **Final remarks on the nanoprobe**
CARNAÚBA will tackle questions in areas of fundamental importance to science, as in life, geological, environmental and materials science. Its nanoprobe will allow answering many questions regarding the nature of these heterogeneous samples, such as local composition, chemistry, atomic structure, crystal orientation, strain, among other important characteristics, aiming to go down to spatial resolution of few nanometers. When the sample is raster scanned in front of the beam to form an image, the resolution is directly related to the spot size, which depends on energy (Fig. 3-Left). Techniques collecting the transmitted beam through the sample, the fluorescence or the diffraction will be available at the beamline with that spatial resolution. For reciprocal space imaging, resolution depends on the coherent dose on the sample and the flux density is a more relevant parameter (Fig. 3-Right). The attainable resolution will depend on how efficiently the coherent beam is focused into the sample, without too much deforming the wave-front, on stability of the sample to the optics and on the availability of fast area detectors to handle the amount of photons.

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