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DESIGN AND RAY-TRACING OF THE BEATS BEAMLINE OF SESAME*

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Abstract

The European Horizon 2020 project BEAmline for Tomography at SESAME (BEATS) has the objective to design, procure, construct and commission a beamline for hard X-ray full-field tomography at the SESAME synchrotron in Jordan. In this paper we present the raytracing simulations performed to quantify the performance and verify the optical design of the beamline. The specifications of a vertically-deflecting double multilayer monochromator are investigated comparing multilayer mirrors with different meridional slope error. The use of a pinhole in the beamline Front-End (FE) acting as a secondary source with enhanced spatial coherence is discussed for phase-contrast applications. We anticipate that the BEATS beamline will fulfill the needs of a heterogeneous community of users of X-ray tomography at SESAME.

INTRODUCTION

The BEATS beamline will operate an X-ray micro tomography station serving a broad user community. The scientific case of the BEATS beamline is the result of close interactions with the scientific communities of current and potential synchrotron users in the SESAME region. Special emphasis is given to the regional aspect, taking stock of existing research contributions from the region. Four key areas for the scientific case for BEATS in the SESAME landscape are identified:

- Archaeology and Cultural Heritage – This includes the study of archaeological materials such as human, plant or animal remains and artefacts of animal bone, antler and teeth.
- Health, Biology and Food – Research in bone and dentistry; in vitro imaging of the brain vascular and neuronal network and of other organs such as the eye, heart, lung and liver; musculoskeletal and soft tissue imaging; bio mineralisation; entomology; food science.
- Material science and Engineering – Study and development of light and composite materials for construction and transport engineering; energy materials research
- Geology and Environment – Research in soil and rock characterization.

Applications within other domains as well as the possibility to provide services to industrial and private sector users are also envisaged.

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BEAMLINE DESIGN

The design of the beamline allows for a variety of operation modes and ensures sufficient photon flux density in filtered white beam or monochromatic beam from 8 keV and up to 50 keV. The broad energy range and required high photon flux is achieved by a 3 T wavelength shifter insertion device (ID) installed on one of SESAME's short straight sections. The beamline can work with either monochromatic or filtered white beam, with minimum energy tunable by absorbers in the FE. The beam size at the sample position and the propagation distance between sample and detector can be varied displacing the rotation and detector stages along the beam path. For measurements requiring high sensitivity and spatial coherence of the beam (e.g., for phase-contrast tomography), the beamline FE slits are partly closed to define a smaller, secondary source with higher spatial coherence.

Layout

The beamline FE comprises photon absorbers and stoppers, a mask defining a useful beamline aperture of 1.8 $mrad$ (h) by 0.36 $mrad$ (v), a CVD diamond window separating the machine and the beamline vacuum, filters and primary slits. The main optical component is a Double Multilayer Monochromator (DMM) placed outside of the SESAME storage ring tunnel in a dedicated optics hutch. The experimental station is located approximately 45 m from the photon source and comprises secondary slits, a linear fast shutter allowing to reduce exposure of delicate samples [1], a high precision sample positioning and rotation stage, and two full-field detectors based on scintillating screens and sCMOS sensor cameras mounted on a common granite stage [2].

Raytracing

The BEATS optical design is verified with simulation tools included in the OASYS suite [3]. Raytracing calculations are performed in ShadowOui, while power profiles are computed using XOPPY. Software and notebooks for the reproduction of this work are available on Zenodo [4].

Heat Load

The beam power density is calculated for each beamline component sustaining the white beam during operation or possibly in direct sight of the white beam with the OASYS *Wiggler Radiation* widget [5]. The power density profile of the incoming or absorbed beam is used as input for thermal verification with commercial Finite-Element software. Due to the position of absorbers and apertures in the storage ring

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and beamline FE, a portion of dipole emission can enter the beamline. Therefore, for the calculation of the power density profiles on the first two beamline apertures (crotch absorber and fixed mask) the contribution from the upstream and downstream bending magnets is considered in addition to the emission of the BEATS wavelength shifter. For simulations in XOPPY, the magnetic field profile of the BEATS ID is modified to include part of the dipole field as shown in Fig. 1. For all components after the fixed mask, only the ID contribution is considered. The heat load expected on the main beamline components is reported in Table 1.

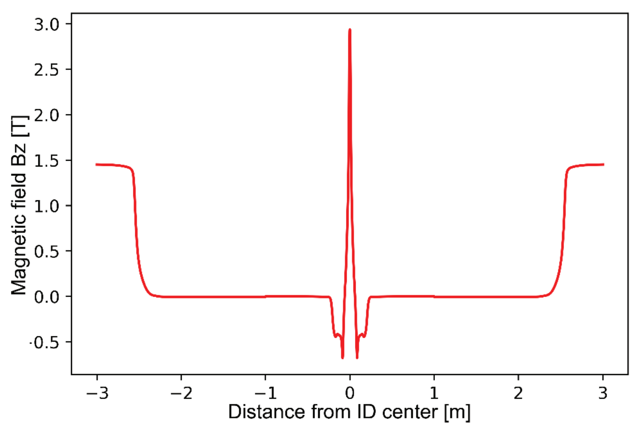

Figure 1: Magnetic field profile modified for simulation in XOPPY considering the BEATS wavelength shifter and the upstream and downstream dipoles.

Table 1: Maximum Power and Power Density on Beamline Components Illuminated by the White Beam

Component	Position $[m]$	P $[W]$	P density $[W/mm^2]$
ID	0.0	857	
Absorber	4.1	4300	20.4
Fixed mask	5.9	271	9.7
Photon shutter	7.6	134	5.2
Window 1	9.0	134	3.7
Filters	11.0	94	1.9
DMM M1	15.1	94	1.0
Combined stopper	94.0	271	0.6
Window 2	37.9	94	0.2

Double Multilayer Monochromator Design

A double-bounce, vertically-deflecting DMM is modelled as a series of two Shadow *Plane Mirror* widgets. The surface and reflectivity of each multilayer is modelled with the Shadow *PreMLayer* PreProcessor. Discrete multilayer surface errors are simulated by external splines with slope error along the beam axis varying between 0.1 and 0.5 μrad (RMS). Modified surfaces are generated with the Shadow PreProcessor - *Height Profile Simulator* widget. The slope error perpendicular to the beam axis is kept constant at 20 μrad RMS, and fractal profiles are chosen (Fig. 2). Plots of the positions of both multilayer mirrors at different working energies are generated for varying bilayer composition and d-spacing. DMM configurations with independent pitch cradles or a common, pseudo-channel-cut layout are investigated.

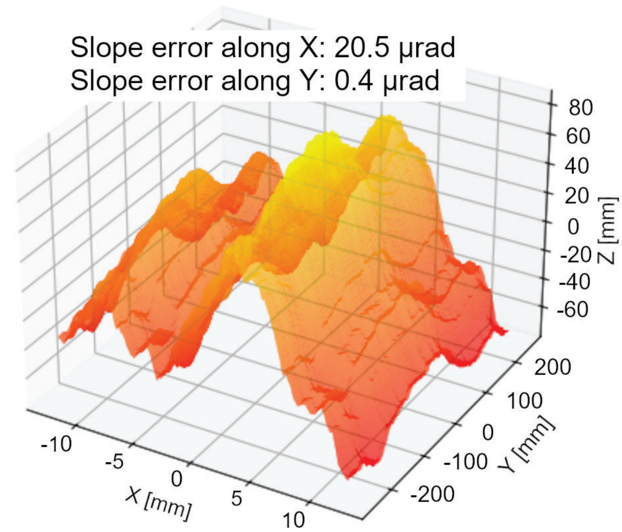

Figure 2: Example of modified multilayer surface: the Y-axis corresponds to the beam path and the X-axis is perpendicular to the beam.

Secondary Source and Coherence Length

Owing to the electron optics of the SESAME storage ring, the BEATS ID generates an X-ray source almost 2 mm in width. Consequently, the beam spatial coherence is limited. To allow for propagation-based phase contrast tomography requiring a certain degree of spatial coherence, the FE slits can be closed to generate a horizontal aperture acting as a smaller and coherent secondary photon source. A comparison of the transverse coherence length at 20 keV with that of other tomography beamlines is shown in Table 2. The transverse coherence length is calculated as:

$$l_{coherence} = \frac{2\lambda d}{\sigma_x} \tag{1}$$

where d is the distance between source and sample, λ is the wavelength (0.62 $\AA$) and σ_x is the FWHM horizontal photon source size [6].

The reduced beam size available with FE slits closed can be calculated as $2\eta_x d$ where η_x is the effective beam half-divergence behind an aperture of size a:

$$\eta_x = \frac{\sqrt{(\frac{\sigma_x}{2})^2 + (\frac{a}{2})^2}}{d} \tag{2}$$

The effect of closing the FE slits on both the available white beam size and flux for experiments is investigated through raytracing simulations.

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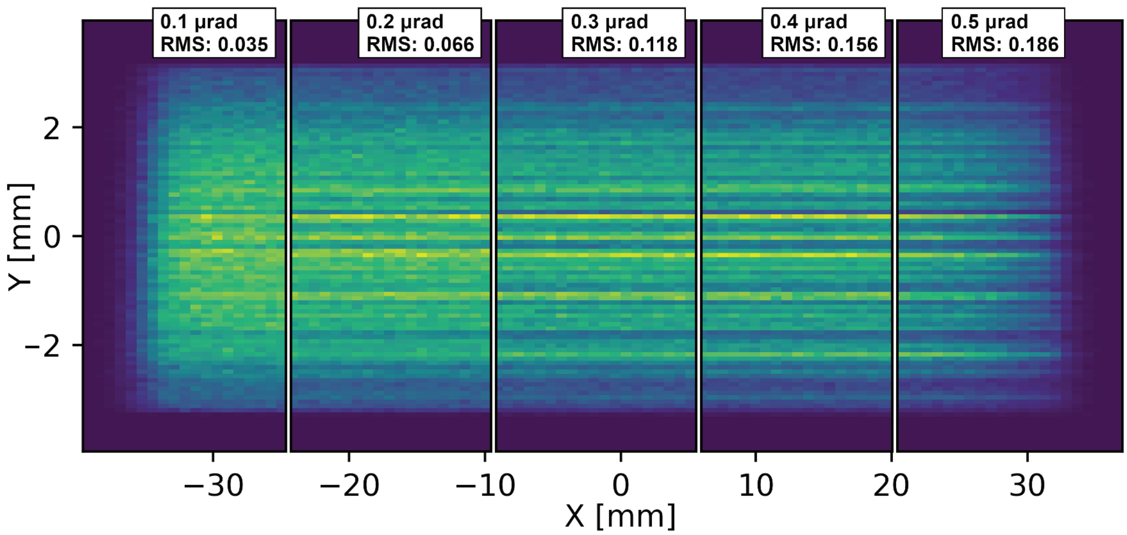

Figure 3: Monochromatic beam flat field snapshots at the sample position (43 m from source) for different multilayer mirrors slope errors. $[W/B_4C]_{100}$ bilayers with a d-spacing of 3.0 nm coated on $500 \times 25\ mm^2$ mirror surfaces are considered. The grazing angle is optimized for an energy of 45 keV ($\theta = 0.274°$). 16×10^6 rays are used for Monte Carlo simulations.

Table 2: Transverse Coherence Length at 20 keV; Comparison of BEATS with other Beamlines

Beamline	d $[m]$	σ_x $[\mu m]$	$l_{coherence}$ $[\mu m]$
ID19@ESRF	145.0	25	720.0
TOMCAT@SLS	34.0	140	30.2
SYRMEP@Elettra	23.0	197	14.5
BEATS	43.0	1978	2.7
BEATS - Slits @ 0.5 mm	34.6	500	8.6

RESULTS

The expected white beam flux delivered through a square millimeter at the sample position is as high as $1 \times 10^{10}\ Ph/s/mm^2$ in 0.1 % of the source bandwidth, for a maximum usable beam size of $72 \times 15\ mm^2$. With both multilayers, the expected energy resolution of the monochromatic beam is 3 %, for a total monochromatic photon flux at 20 keV of $3 \times 10^{11}\ Ph/s/mm^2$ through one square millimeter at the sample. Simulated monochromatic beam profiles at the sample are shown in Fig. 3 after double reflection by two multilayers with varying mirror surface slope error. The quality of the flat field deteriorates for mirror slope errors > 0.2 μrad. When the FE slits are closed to produce a secondary photon source, the beam size is also reduced, limiting the horizontal field of view for phase contrast imaging to 10 mm or less (Fig. 4). The reduction in photon flux density at the sample position when the FE slits are closed to 500 μm is estimated to be of the order of 70 %.

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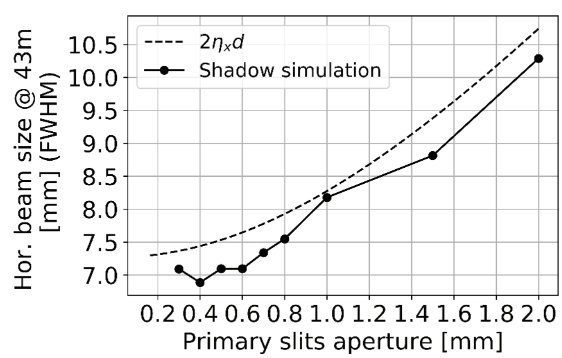

Figure 4: Horizontal beam size at the sample position when the FE slits aperture is reduced.

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