



SESAME

29 April 2021

Report on ML slope error

BEATS - BEAmline for Tomography at SESAME

Summary

Raytracing of the BEATS beamline Three-Pole-Wiggler source and Double Multilayer Monochromator. Two 500mm-long plane mirrors with modified surface slope error and PreMLayer reflectivity are considered for the DMM. A W/B4C stripe with 100 MLs and (graded) d-spacing of 3 nm is considered at beam energy of 45 keV. Beam profiles at the sample position are shown for 0.1, 0.2, 0.25, 0.3, 0.35, 0.4 and 0.5 μrad mirror slope error. The quality of the flat field is affected already for slope errors $\geq 0.25 \mu\text{rad}$.

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Version history:

- Ver 1.0 BEATS TDR
- Ver 2.0 Changed substrate size based on feedback from CM and companies
- Ver 3.0 Feedback CM, RB, JRH and RM
- Ver 4.0 Increased ML length to 500mm; W/B4C stripe d-spacing: 3nm
Added substrate slope error simulations

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0.1 Resources

- BEATS raytracing codes can be found on GitHub [here](#).
- Figures (e.g. beam profiles) are stored [here](#).

0.2 Beamline layout

See beamline drawing and beamline functional layout attached.

1 X-ray source - Three Pole Wiggler (3PW)

1.1 Wiggler plots

The magnetic field profile of the BEATS 3PW is shown in Figure 1.

Figure 2 shows the electron beam trajectory.

Figure 3 shows the expected 3PW flux spectrum.

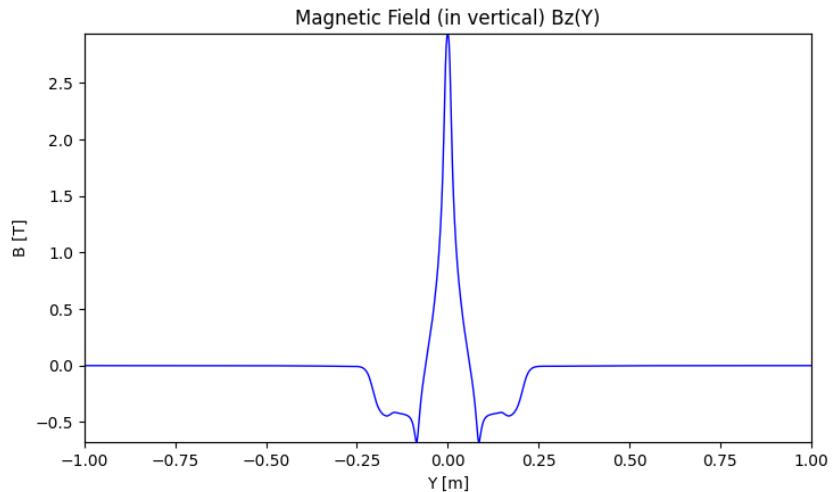


Figure 1: BEATS 3PW magnetic field profile.

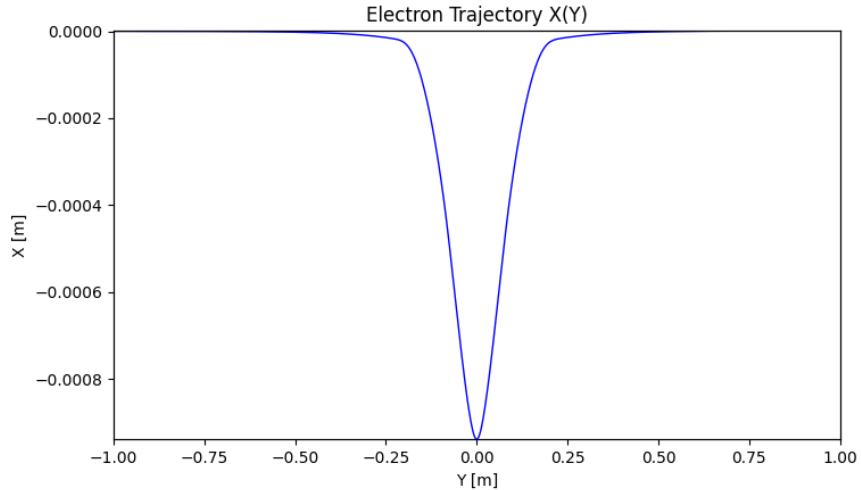


Figure 2: BEATS 3PW electron beam trajectory.

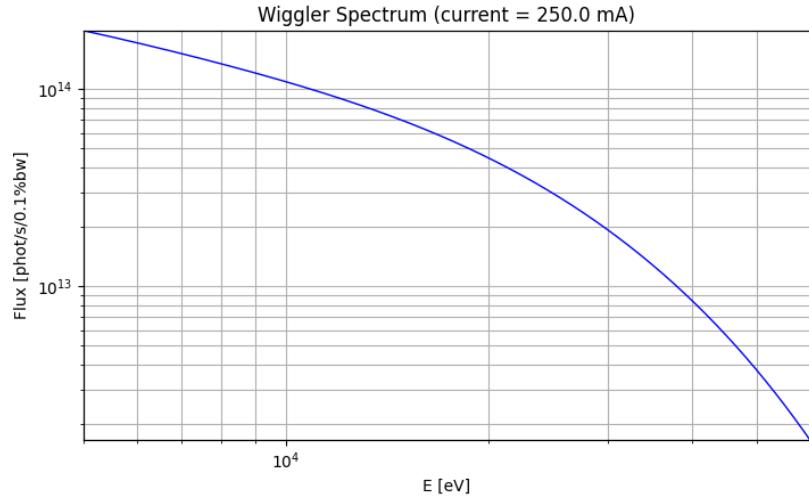


Figure 3: BEATS 3PW spectrum.

1.2 Source size and divergence

Figure 4 shows the BEATS source size. The source has an offset of almost 1mm. Plots of the horizontal and vertical photon source size and divergence are shown in 5.

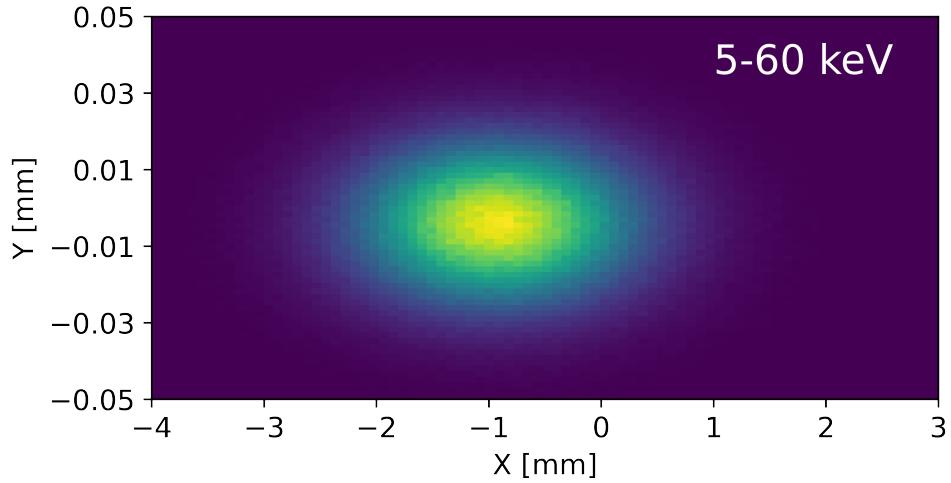


Figure 4: BEATS 3PW photon source snapshot.

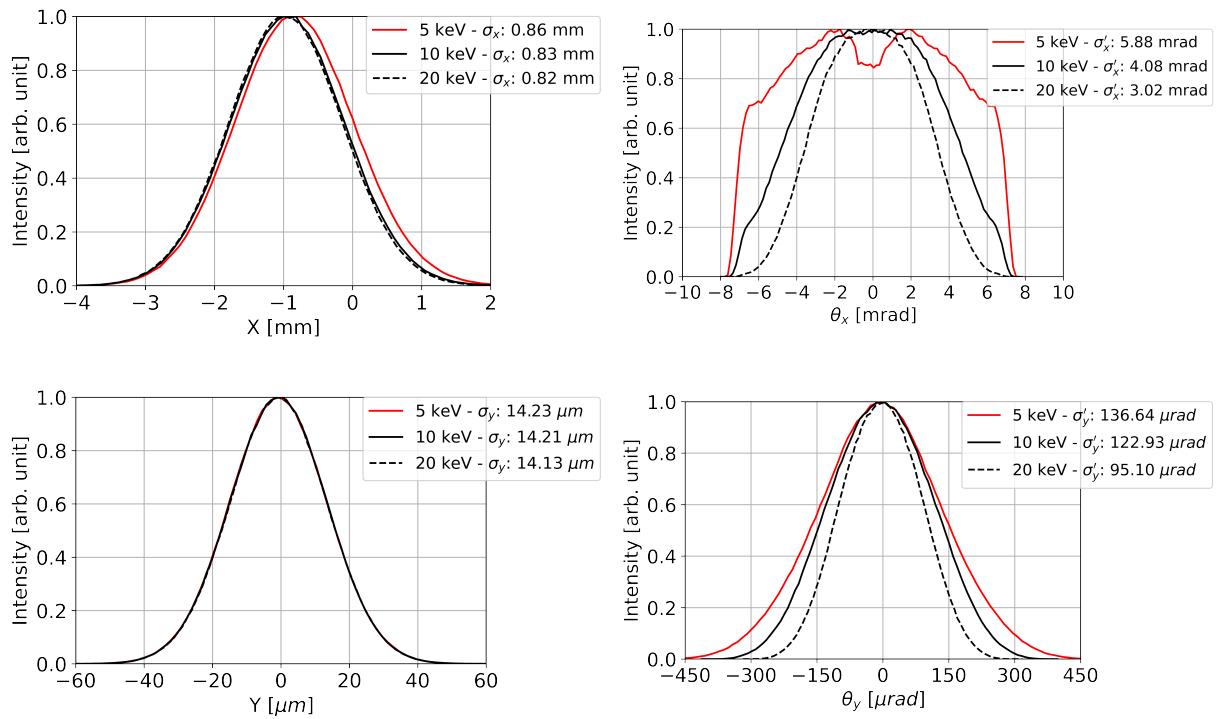


Figure 5: Photon source size and divergence of the BEATS 3PW at 5, 10 and 20 keV.

2 Double Multilayer Monochromator (DMM)

Deflection	Vertical
Distance from source (1st ML)	15.165 m
Beamline aperture	1.8 mrad \times 0.4 mrad (Hor. \times Ver.)
Beam size @ 1st mirror	29 mm \times 6 mm (Hor. \times Ver.)
Working energy	8 – 50 [keV]
ML length	500 mm
Distance between MLs	510 mm
Offset (variable)	Min. 4.2 – Max. 16.0 [mm]
Theta (Bragg angle)	-0.5 to +2.5 [deg]
Bragg resolution	0.5 μ rad
Max. power on 1st mirror	133 W

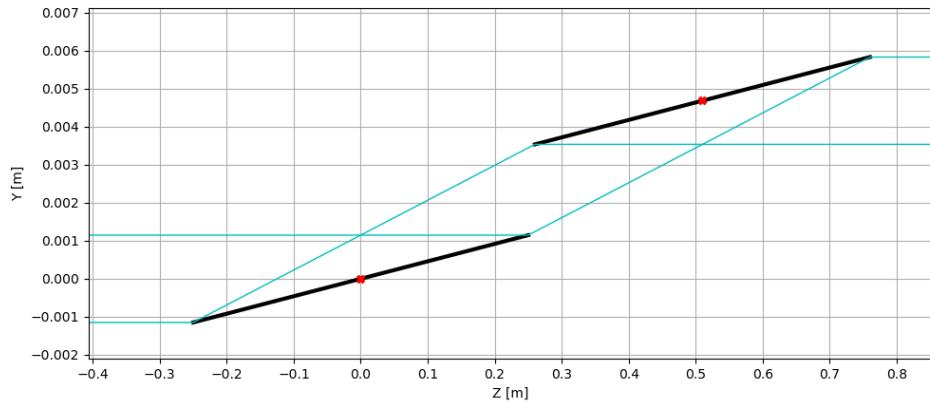


Figure 6: d-spacing: 3 nm; E: 45 keV; Grazing: 0.263 deg; offset: 4.68 mm.

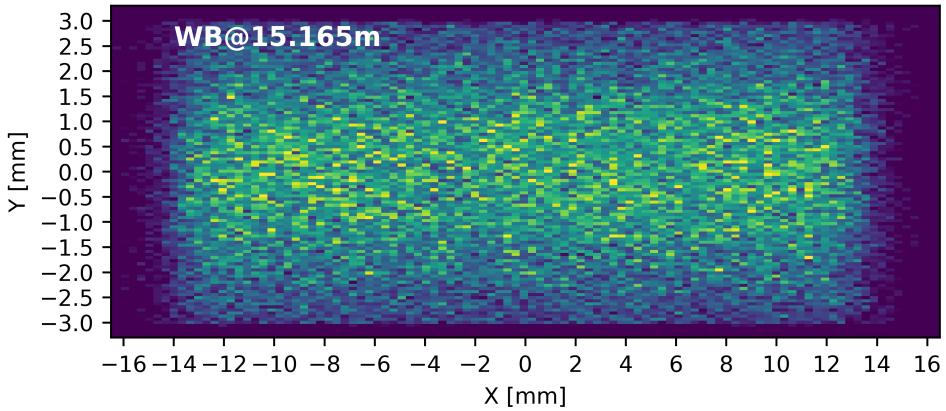


Figure 7: White beam snapshot at 15.165 m from source (center position of ML1).

2.1 Substrates

The ML length was increased to 500 mm. A drawing of the proposed substrate size is attached. The substrate size and optical quality (tentative) are reported in Table 1.

Substrate dimension	500 mm × 70 mm × 60 mm (see drawing attached)
Coated area	500 mm × 25 mm (2 stripes)
Surface roughness	< 0.3 nm rms
Slope error along Z	≤ 0.3 μrad rms
Slope error along X	< 20 μrad rms

Table 1: BEATS DMM substrates.

2.2 ML coatings

Following the increase in ML length to 500 mm the d-spacing of the high-energy stripe is changed back from 2.5 nm to 3.0 nm. This gives approx. +50% int. reflectivity (dE/E increases from 2.3% to 3.2%). Thanks to the increased mirror length, the useful vertical part of the beam is intercepted even at minimum grazing and even with a d-spacing of 3.0 nm. Coating specs of the two ML stripes are given in Table 2.

	STRIPE 1 [W/B ₄ C] ₁₀₀ – d3.0nm]	STRIPE 2 [Ru/B ₄ C] ₆₅ – d4.0nm]
Materials	W/B ₄ C	Ru/B ₄ C
d-spacing [nm]	3.0	4.0
d-spacing gradient along Z (O.A. 500 mm)	3.297 % (0.00659 % / mm)	
N. bilayers	100	65
Duty cycle γ	0.5	0.5
Energies [keV]	20 – 50	8 - 22
dE/E	3.2 %	3.1 %
Coated area	480 mm × 25 mm	
Theta (Bragg angle) [deg]	0.23 – 0.59	0.41 - 1.00

Table 2: BEATS multilayer coatings.

Multilayer Parameters	
Output file (for SHADOW/trace):	<code>#C100_d30_gradient.dat</code>
Min Energy [eV]	1000.0
Max Energy [eV]	100000.0
Material (substrate) (element or formula)	Si
Density (substrate) [g/cm ³]	2.33
Material (even sublayer) (element or formula)	W
Density (even "bottom" sublayer) [g/cm ³]	19.3
Material (odd sublayer) (element or formula)	B4C
Density (odd "top" sublayer) [g/cm ³]	2.52
Multilayer Parameters	
Bilayer thicknesses graded along the dep No (Constant)	
Number of bilayers	100
bilayer thickness t [Å]	30.0
gamma ratio [t _{even} /(t _{odd} +t _{even})]	0.5
Roughness even layer [Å]	3.1
Roughness odd layer [Å]	3.3
Bilayer thicknesses/gamma graded along the surf thickness graded (from quadratic fit)	
Fit bilayer tr(v)/t(v=0) vs v: zero-order coefficient (constant)	1.0
Fit bilayer tr(v)/t(v=0) vs v: linear coefficient (slope)	-6.594e-05
Fit bilayer tr(v)/t(v=0) vs v: 2nd dearee coefficient	0.0
Fit bilayer tr(v)/t(v=0) vs v: 3rd dearee coefficient	0.0

Figure 9: PreMLayer widget settings in Shadow.

2.3 Raytracing

The double-bounce DMM is modelled with two Shadow Plane Mirror widgets in series (Figure 8). ML reflectivity is modelled with a Shadow PreMLayer widget as shown in Figure 9. The mirror surface is modified with Surface Error external splines with varying longitudinal slope error (0.1, 0.2, 0.3, 0.4 and 0.5 μrad RMS). These modified surfaces (10) are simulated with the Shadow PreProcessor - Height Profile Simulator widget. The transversal slope error is kept constant at 20 μrad RMS and fractal profiles are chosen.

Slope error rms in X direction: 20.534462 μrad
Slope error rms in Y direction: 0.200000 μrad
Figure error rms in X direction: 32.136488 nm
Figure error rms in Y direction: 5.450626 nm

Slope error rms in X direction: 20.534462 μrad
Slope error rms in Y direction: 0.300000 μrad
Figure error rms in X direction: 32.136488 nm
Figure error rms in Y direction: 8.175939 nm



Figure 8: Double Multilayer Monochromator in Oasys Shadow.

Slope error rms in X direction: 20.534462 μrad
Slope error rms in Y direction: 0.400000 μrad
Figure error rms in X direction: 32.136488 nm
Figure error rms in Y direction: 10.901253 nm

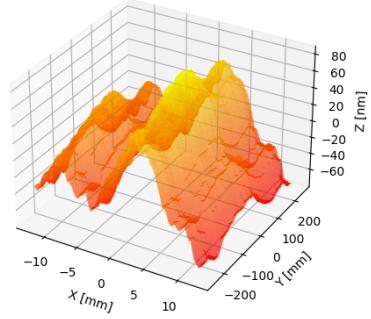
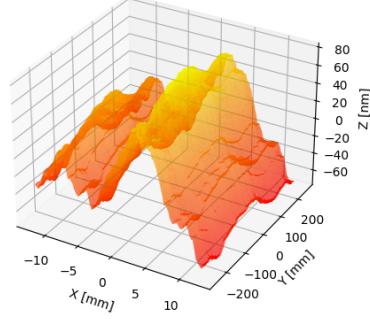
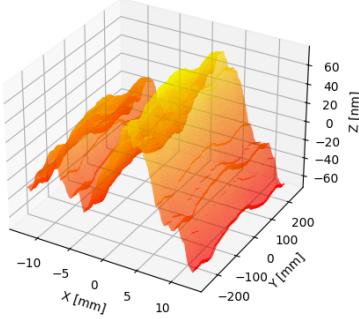


Figure 10: Modified mirror surfaces.

2.4 Substrates slope error

For the comparison of different substrates slope error of this paragraph a total O.A. length of 500 mm is considered.

2.4.1 0.1 urad

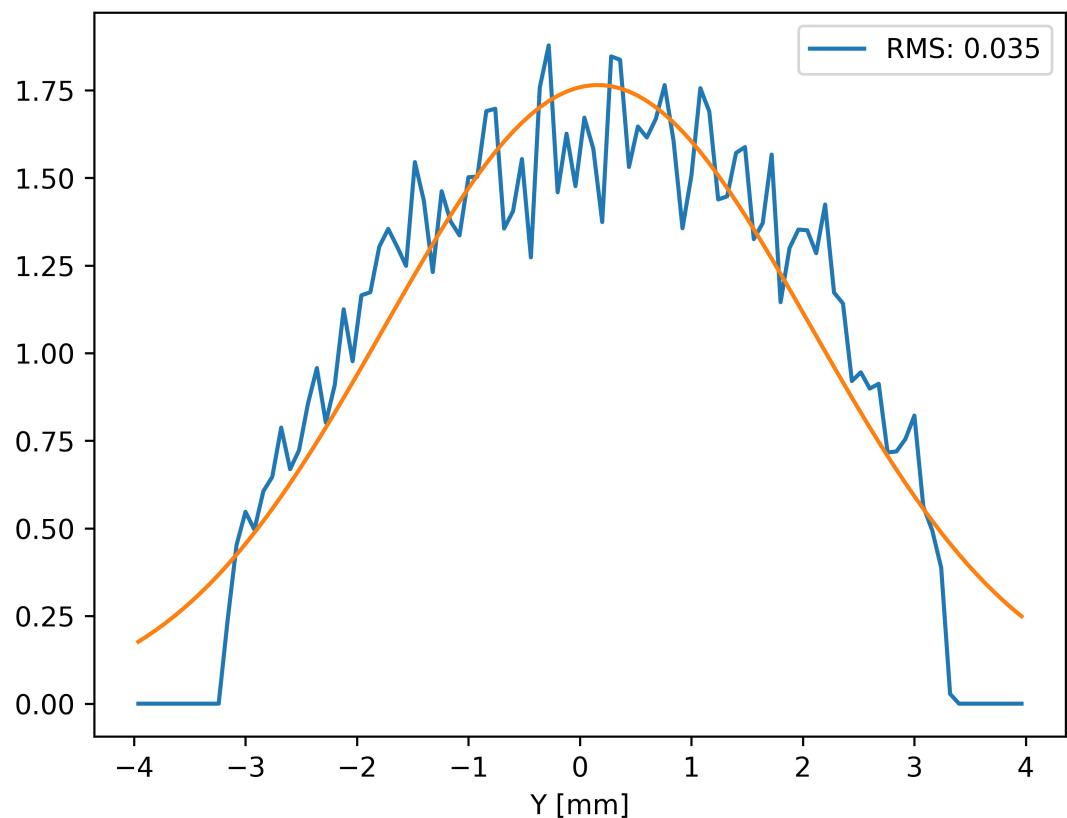
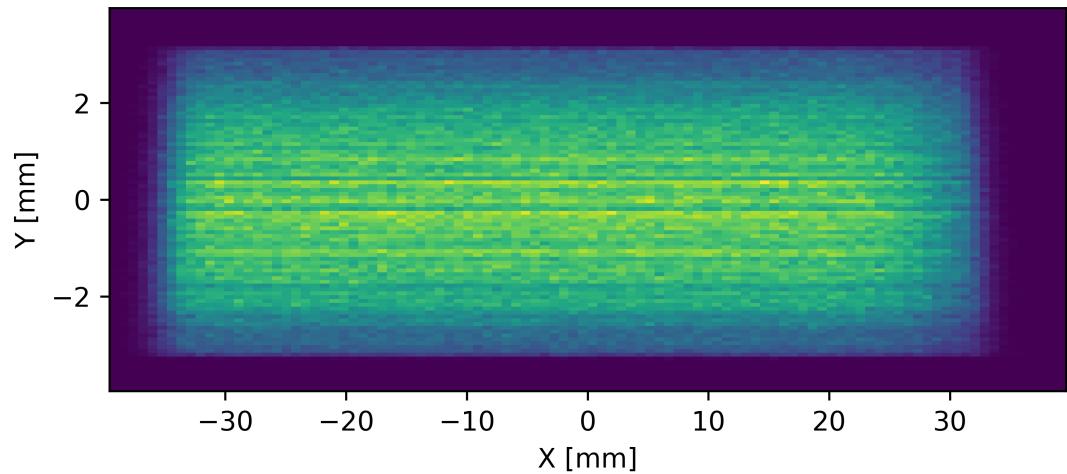


Figure 11: 0.1 urad

2.4.2 0.2 urad

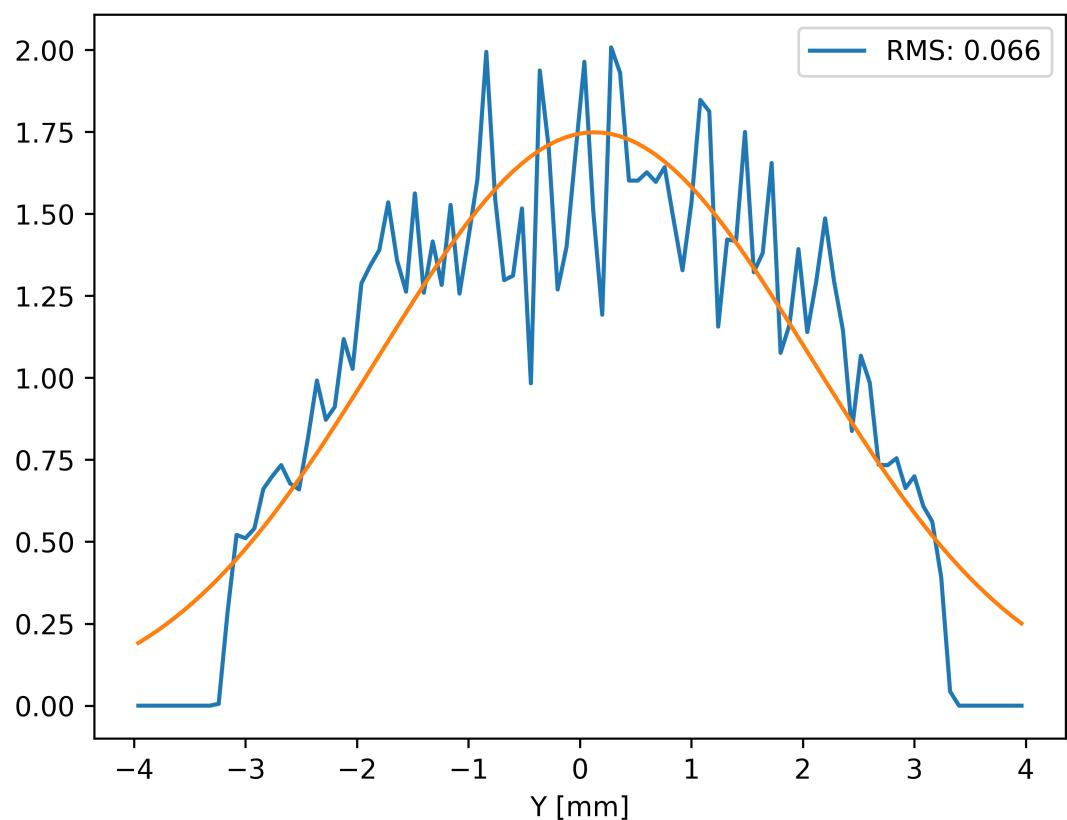
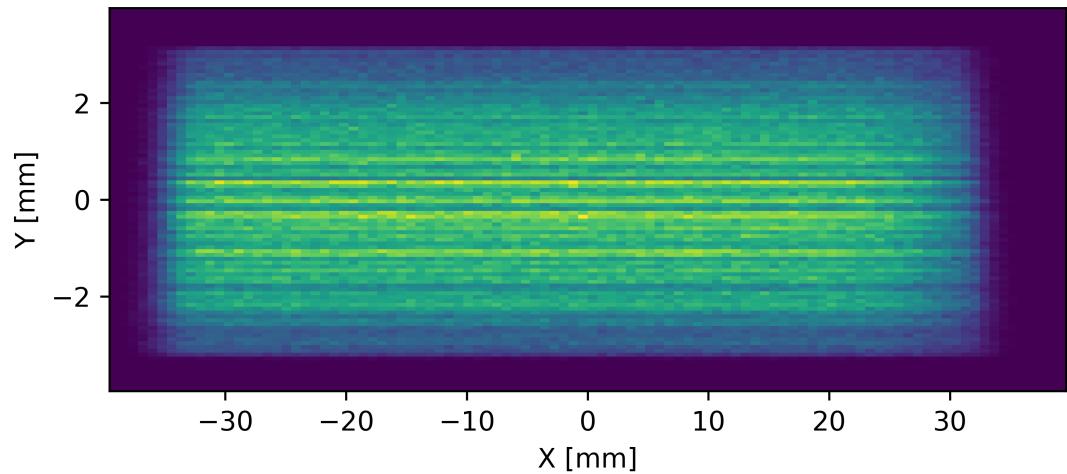


Figure 12: 0.2 urad

2.4.3 0.25 urad

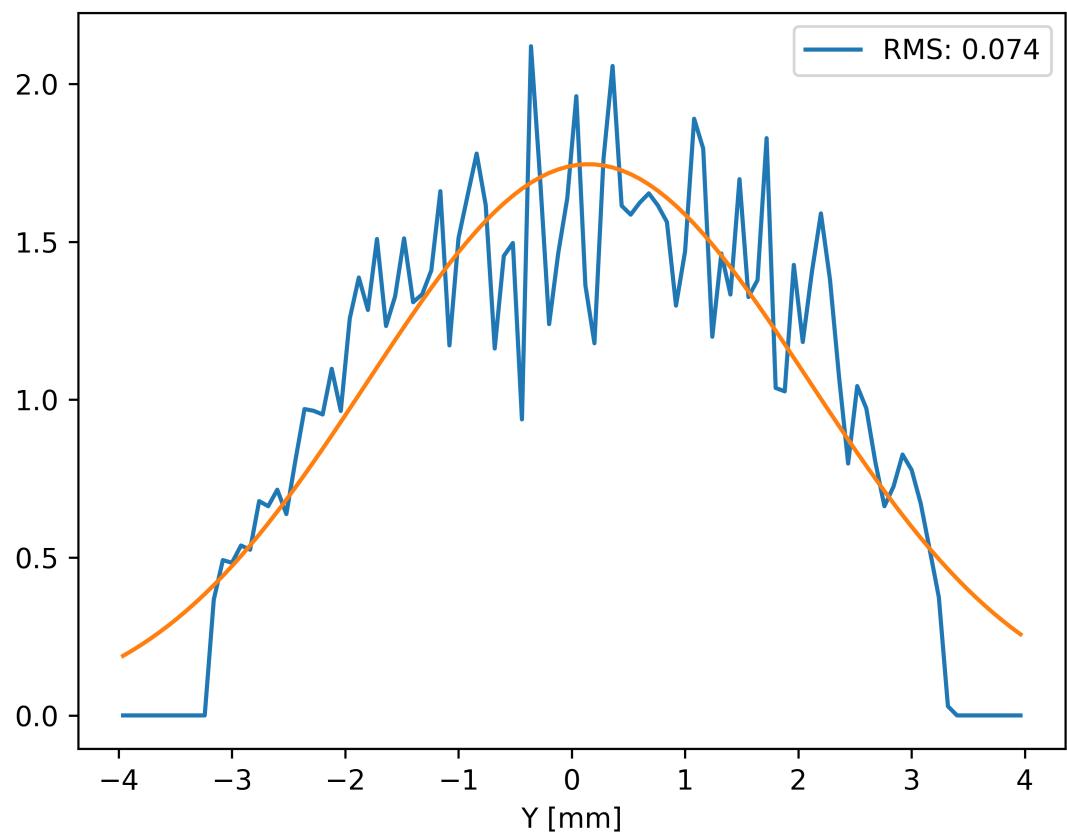
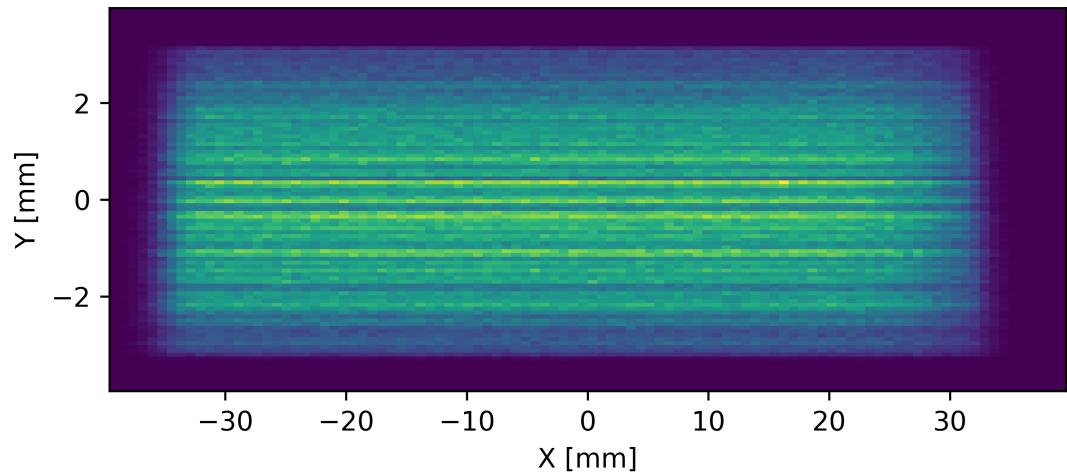


Figure 13: 0.25 urad

2.4.4 0.3 urad

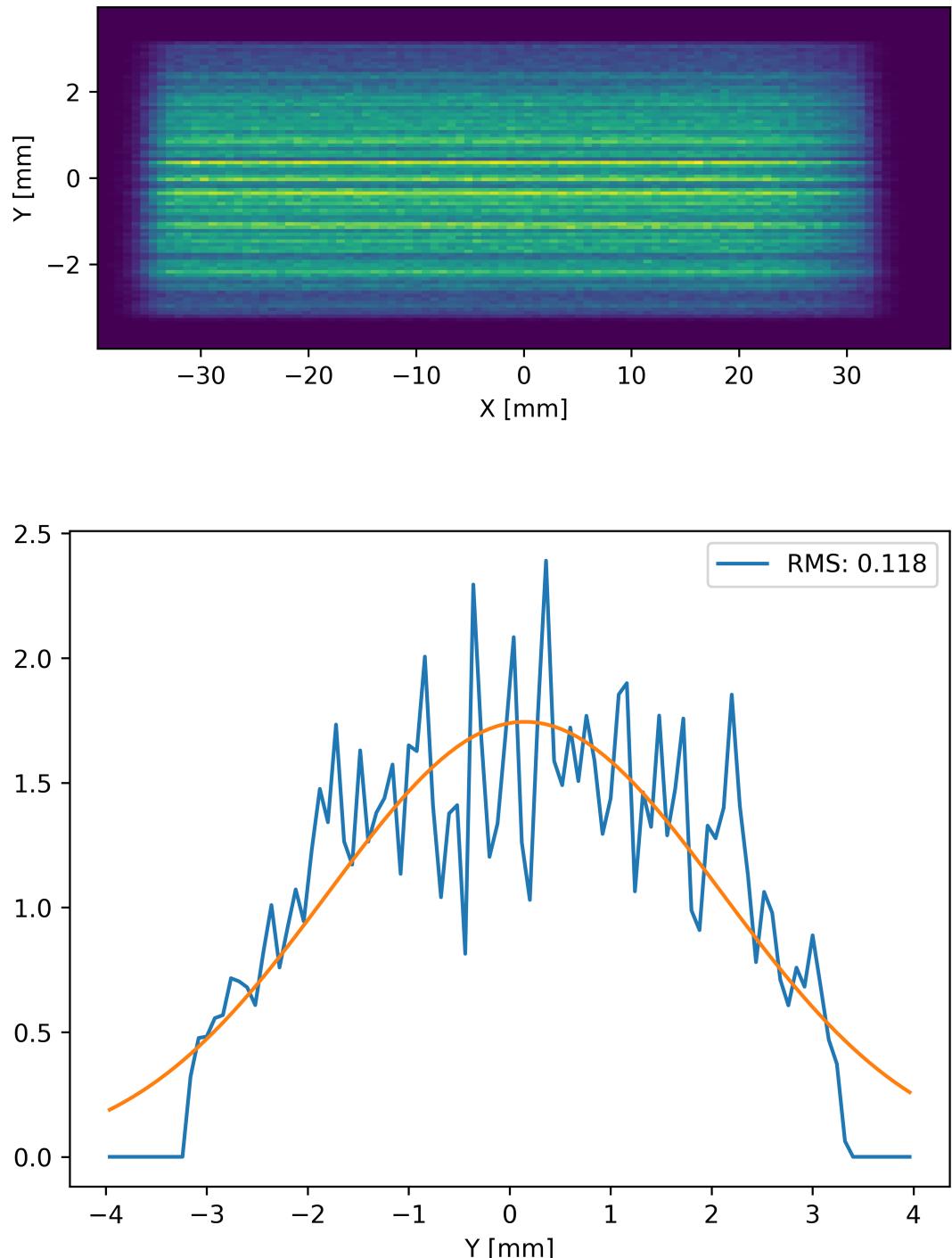


Figure 14: 0.3 urad

2.4.5 0.35 urad

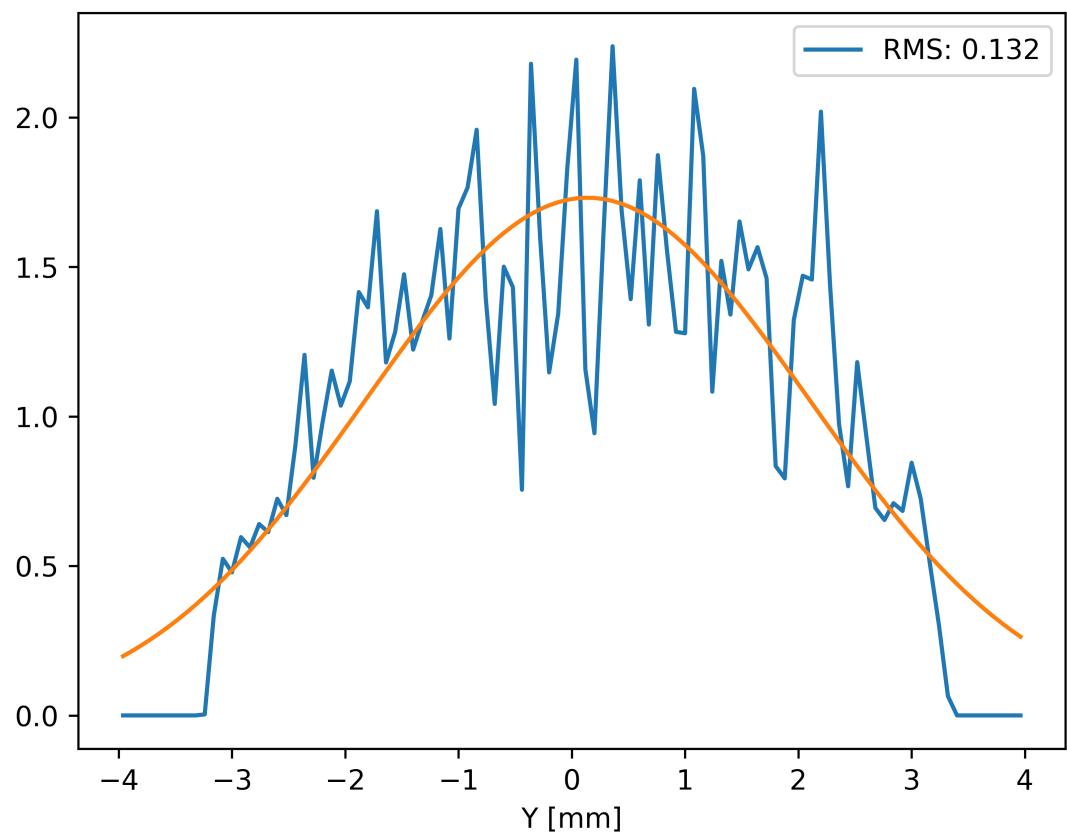
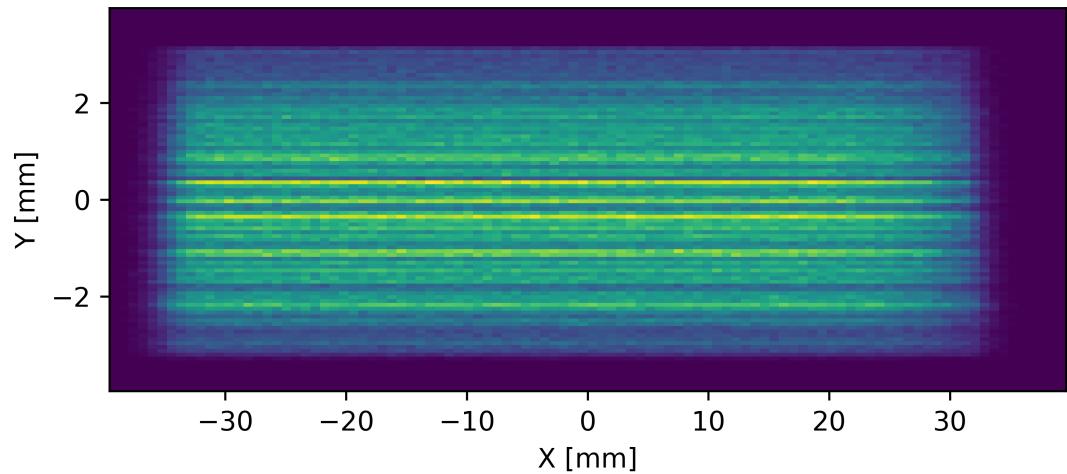


Figure 15: 0.35 urad

2.4.6 0.4 urad

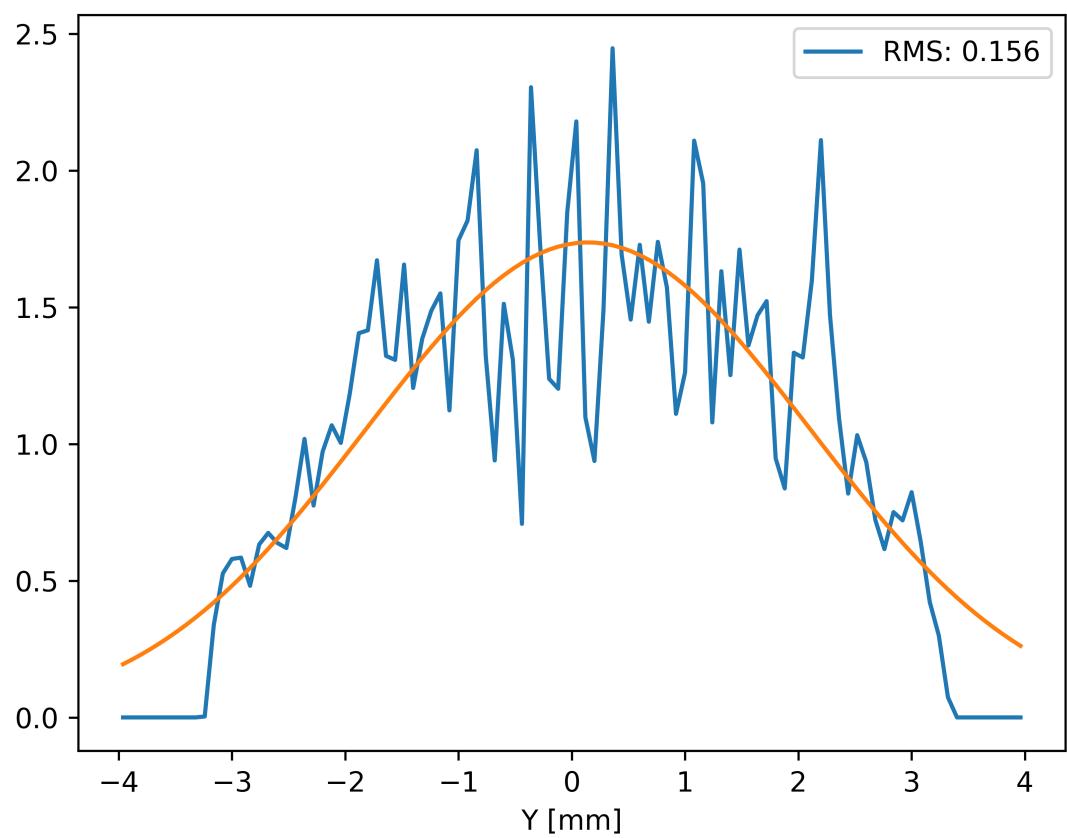
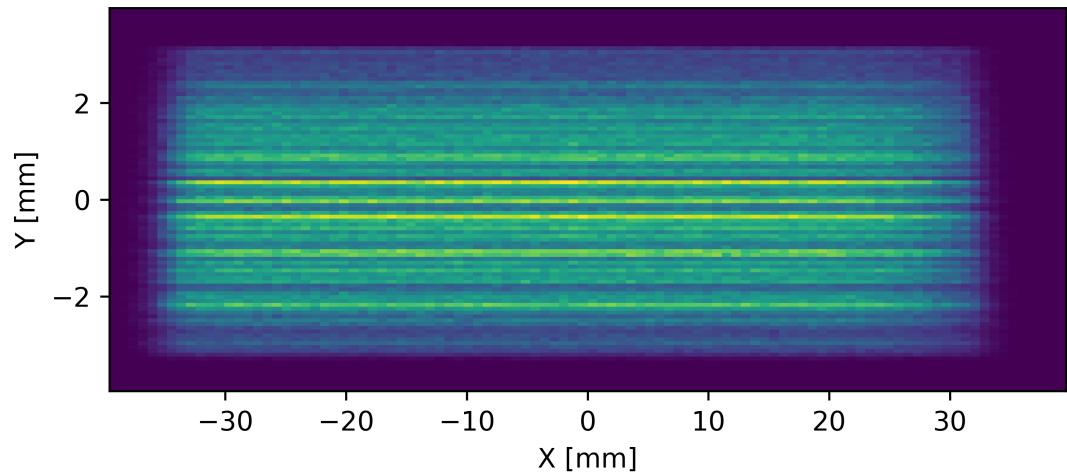


Figure 16: 0.4 urad

2.4.7 0.5 urad

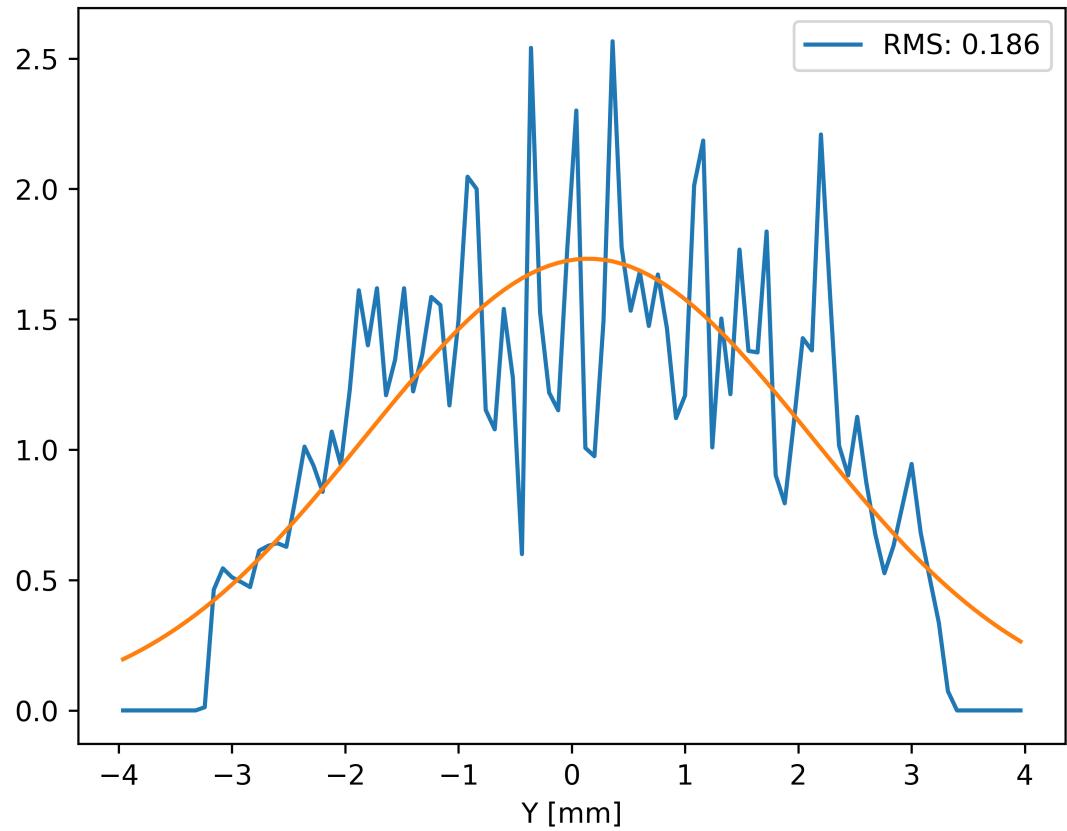
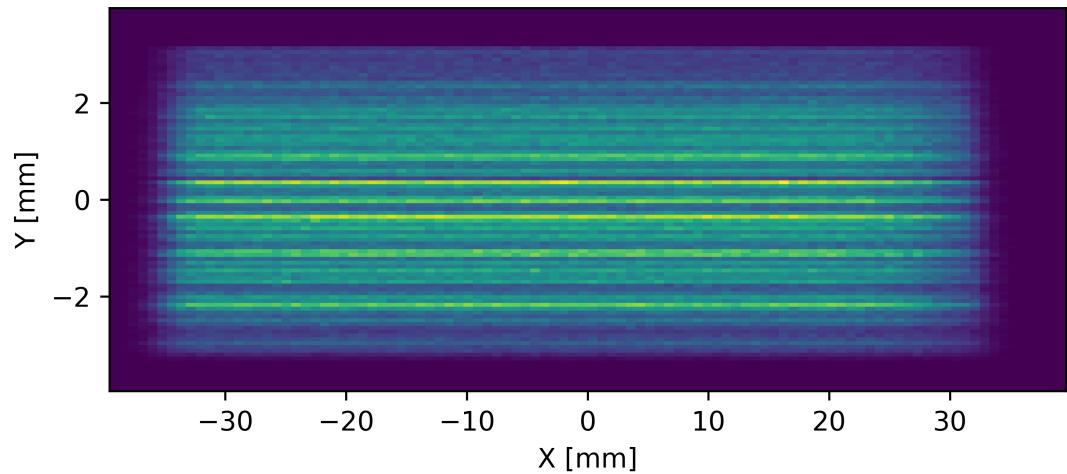


Figure 17: 0.5 urad

2.5 Thermal stability

The thermal stability of ML1 should be verified with FEA simulations considering the white beam colliding with the mirror at the maximum Bragg angle allowed by the Bragg stage motorization (34.9 mrad). The thermal stability of the cooled mask in front of the ML1 profile shall be also verified.

The power density profile at 15.165 m from source is shown in Figure 18. Raw data can be found in the [power profiles source](#).

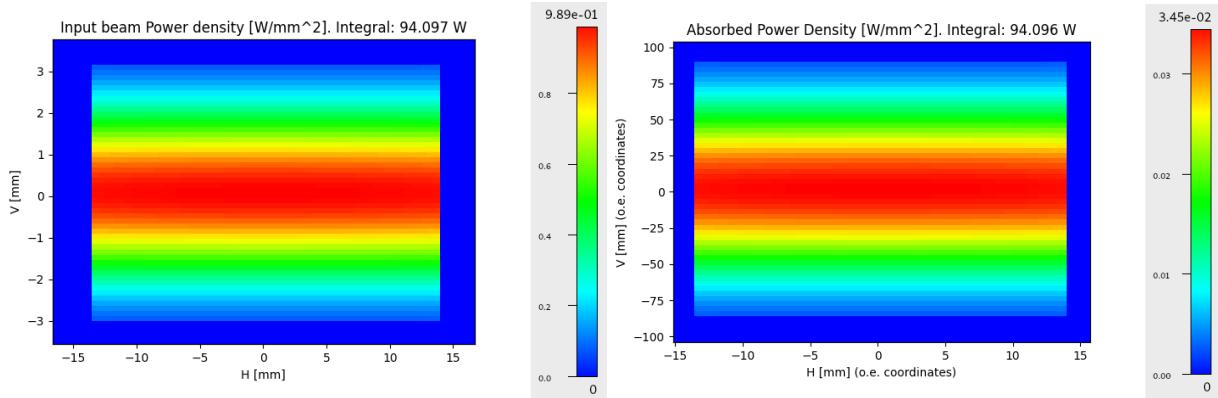


Figure 18: Power density profile at 15.165 m from source (center position of ML1). (LEFT) Input beam. (RIGHT) Absorbed by substrate at maximum grazing (2 deg); reflectivity neglected.