

KB focusing optics for the SQS Scientific Instrument



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WP85, Scientific Instrument SQS
Instrument Scientist

Satellite meeting soft X-ray instruments SQS and SCS
Hamburg, January 24th 2017

Outline

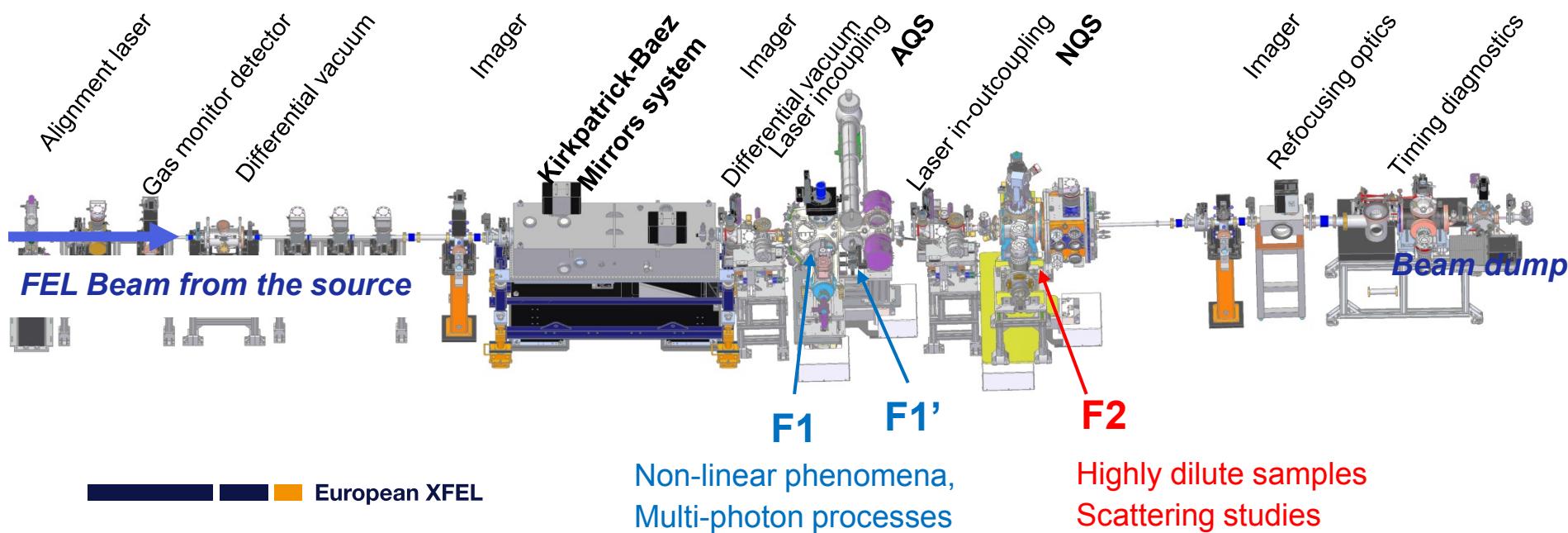
- Focusing system functional specifications coping with
 - Science case
 - Source, beamline, instrument characteristics
- Conceptual and technical solution for the SQS KB system
- Expected performances: results from simulations
 - ray tracing
 - wavefront propagation
- The solution for day one
- Characterization tools

Functional specifications

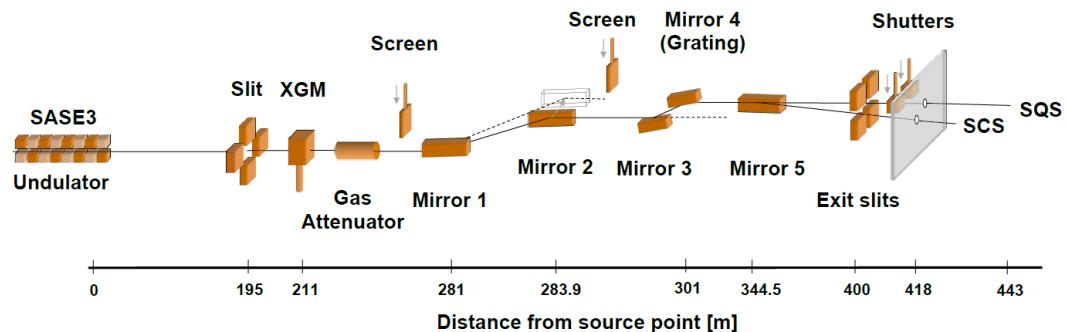
- Focus high power FEL radiation over a broad photon energy range (0.25 – 3 keV)
- Focus it very tightly to obtain conditions for non-linear phenomena
- Focus it very tightly into three (!!) different interaction regions
- In addition: allow for operation of both mono and pink beam operation

SQS Scientific Instrument science cases:

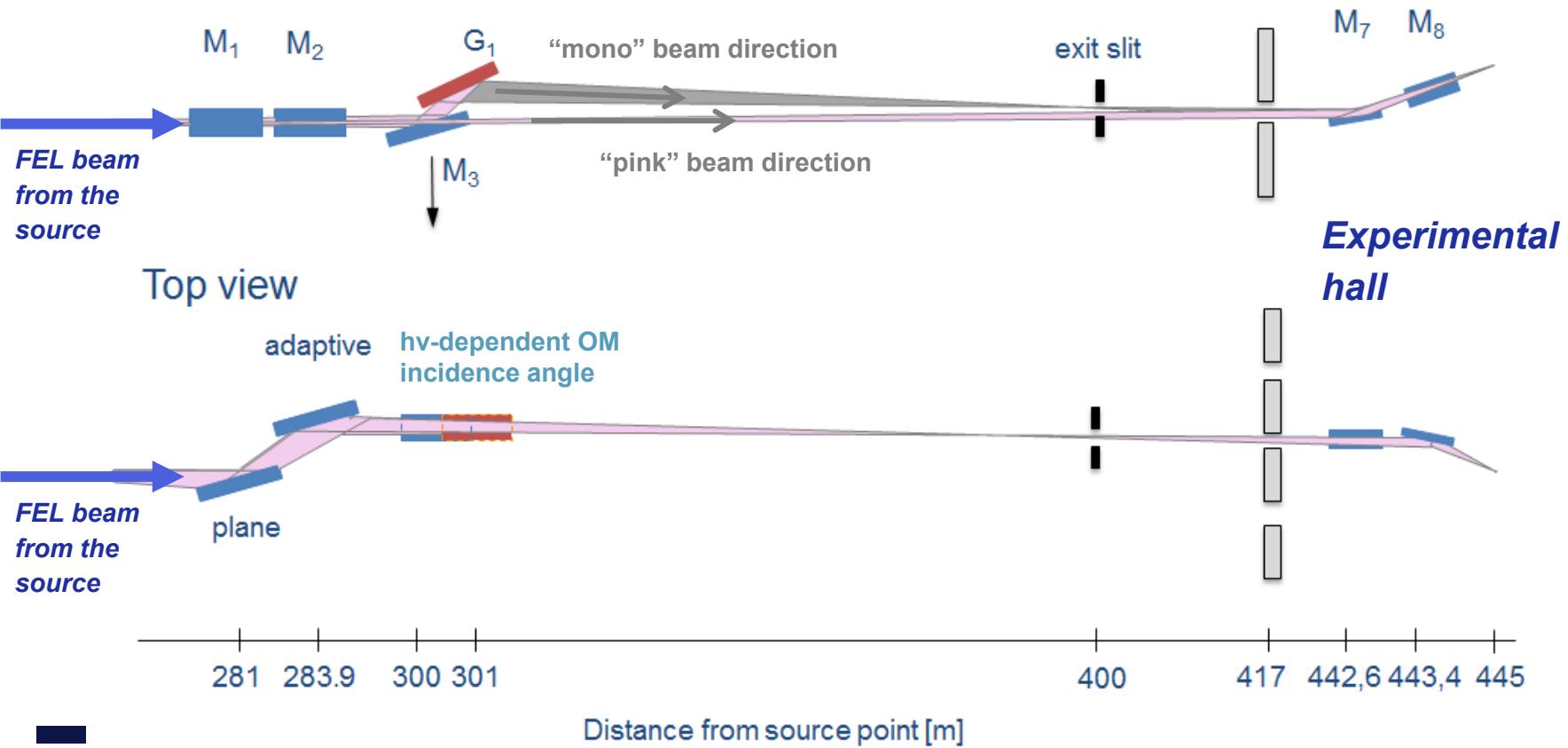
- Non-linear phenomena, multi-photon processes
- Ultra-fast dynamics
- Extremely dilute targets processes with small cross section



SASE3 Optical Layout



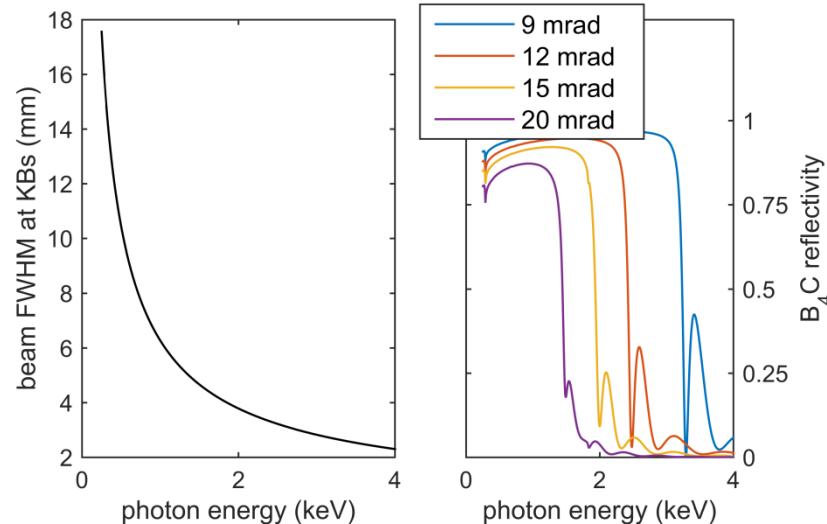
Side view



The solution, conceptually: KB optical system made of two elliptical mirrors that are:

1. Very long
2. With very high surface quality
3. Actively cooled
4. Equipped with mechanical benders to be adaptive

*Why should the mirrors be **that** long?*



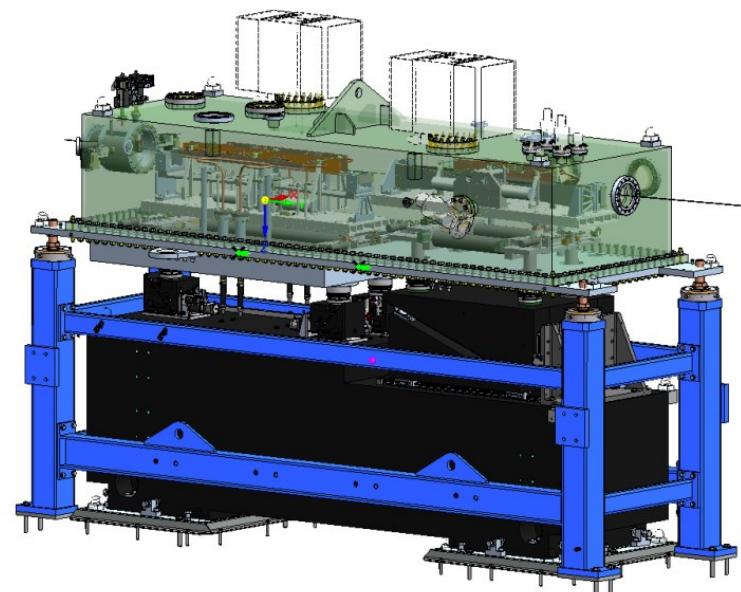
*What does our surface quality requirement (**2nm / 1m**) mean:*



The solution, technically

- Contract awarded to FMB Oxford
 - Super-polished substrates
(subcontractor: JTEC)
 - Vacuum vessel + mechanics
 - installation

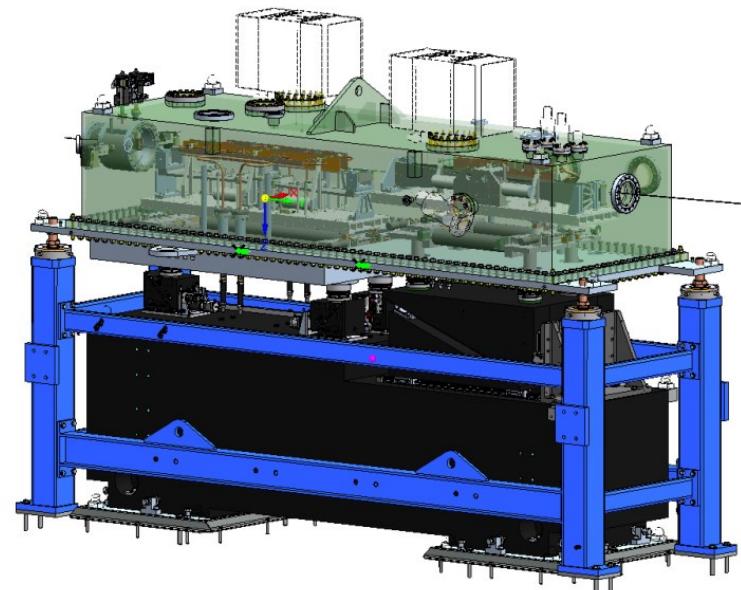
- Current status:
 - Final design released (Dec 2015)
 - Vessel and mechanics under production (ready soon)
 - Grouting plates installed in the experimental hutch
(Jan 2017)



The solution, technically

- Contract awarded to FMB Oxford
 - Super-polished substrates
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 - Vacuum vessel + mechanics
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- Current status:
 - Final design released (Dec 2015)
 - Vessel and mechanics under production (ready soon)
 - Grouting plates installed in the experimental hutch (Jan 2017)
 - Substrates being processed by the subcontractor
 - ▶ Expected delivery Dec 2017
 - ▶ Plan B with spare mirrors for day one under consideration

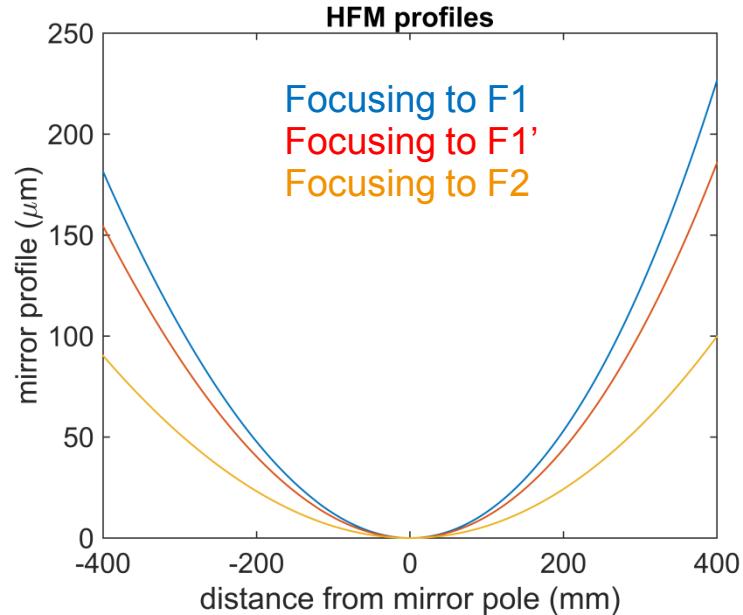


The solution, technically: polishing profiles

- Very steep elliptical profiles!
- Adaptive mirrors with mechanical benders: two end couples induce a curvature in the mirror beam according to the Bernoulli-Euler equation
- **Idea:** polish to profile F1 and bend to the difference between F1 and F1'
- **Problem:** the action of two end couples can only provide a cubic approximation to an ellipse.
- **Solution:** the width of the mirror is modified such that the inertia $I(x)$ is position dependent; for each coordinate it gives the wanted radius of curvature
- Chosen approach:

“polish to F1, lateral shape to F1’”

Howells et al., Theory and practice of elliptically bend x-ray mirrors,
Opt. Eng. 39(10) 2748-2762 (2000)



Bernoulli-Euler equation

$$EI_0 \frac{d^2y}{dx^2} = \frac{C_1 + C_2}{2} - \frac{C_1 - C_2}{L}x,$$

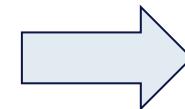
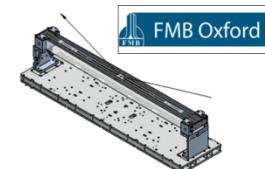
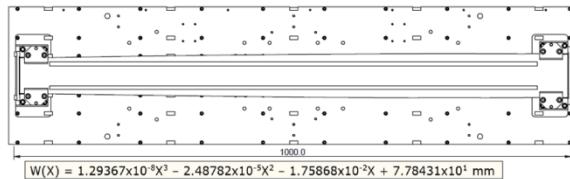
Ellipse curvature

Position-dependent mirror width

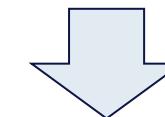
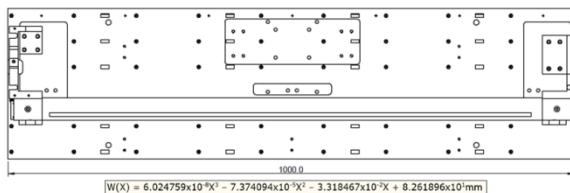
$$b(x) \sim I(x) \sim \frac{(C_1 + C_2)/2 - (C_1 - C_2) \cdot x/L}{\text{"exact ellipse curvature"}}$$

Bending-induced surface error: results from FEA analysis

VFM



HFM



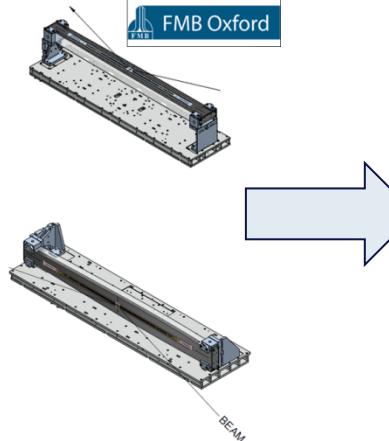
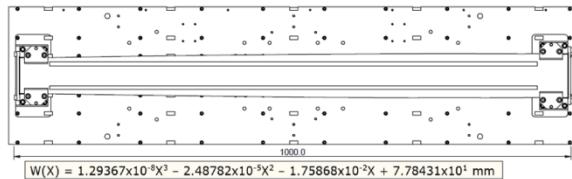
FEA analysis performed by FMB Oxford using ANSYS, estimating:

- optimal clamping force
- optimal end couples for bending to F1' and F2
- Residual error respect to the ideal ellipse (quantified in RMS slope)
- The effect of the thermal load to optimize the design of the bending grooves (see later)

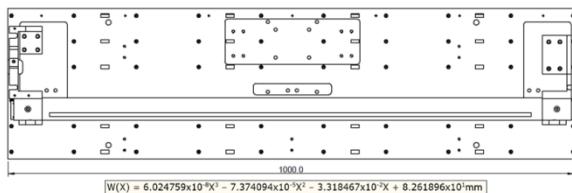
KB	focus	p [m]	q [mm]	Clear aperture [mm]	Error [nrad RMS]
HFM	F1	433,9	1800	800	0
VFM	F1	432,7	3000	800	0
HFM	F1'	433,9	2150	800	15
VFM	F1'	432,7	3350	800	9

Bending-induced surface error: results from FEA analysis

VFM

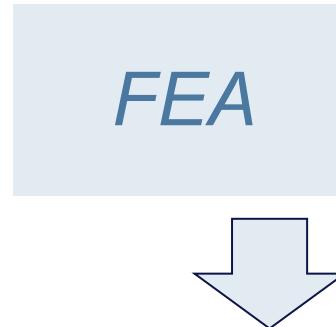


HFM



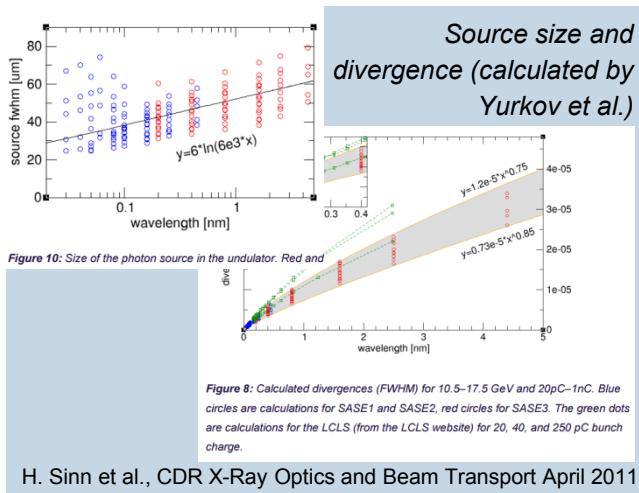
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VFM	F1'	432,7	3350	800	9
HFM	F2	433,9	3832	800	1652
VFM	F2	432,7	5032	800	280

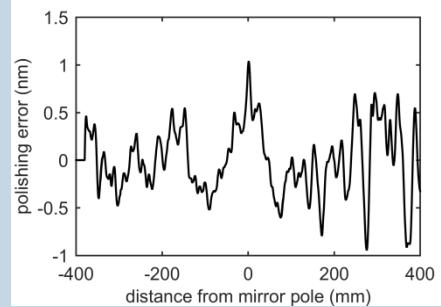
Expected performances: ray tracing simulations



Beamline 3D geometry

Mirrors reflecting surface profiles

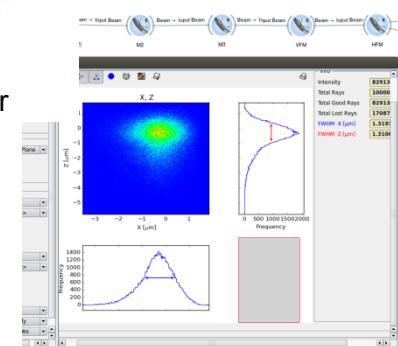
- Polishing error (example from BT mirror prototype, courtesy L. Samoylova)
- Bending error from finite element analysis



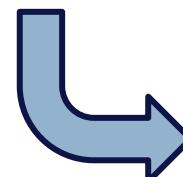
<https://www.elettra.trieste.it/oasys.html>

Including ShadowOui, user interface for Shadow3 (new release of the widely used x-ray optics simulation package)

Credits:
M. Sanchez del Rio (ESRF)
L. Rebuffi (Elettra)



- +
- ✓ Mirrors reflectivity from the CXRO database
 - ✓ Diffraction simulated by a randsinc2 contribution

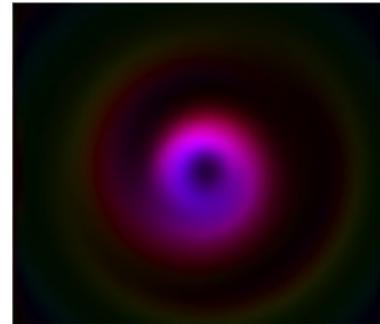


Output:

- ✓ Focal spot profile
- ✓ Rayleigh length
- ✓ Transmission

Expected performances: wavefront simulations

Gaussian beam



WPG

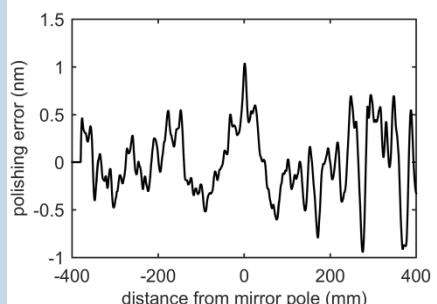
WaveProperGator
with SRW/C++ library

<http://wpg.readthedocs.io/en/latest/index.html>

Beamline 3D geometry (simplified)



Mirrors reflecting surface profiles



- Polishing error (example from BT mirror prototype, courtesy L. Samoylova)
- Bending error from finite element analysis

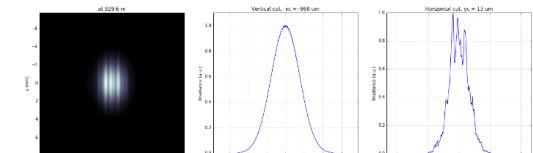


Output:

- ✓ focal spot profile (relative estimate)
- ✓ Wavefront

```
****Imperfect HOM mirror, at KB aperture
FkHx [mm]: 2.89758221191
FkHy [mm]: 3.552090757523
Coordinates of center, [mm]: -0.968117421268 0.0134209978913
stepX, stepY [um]: 13.540103793954389 8.94733192752122
```

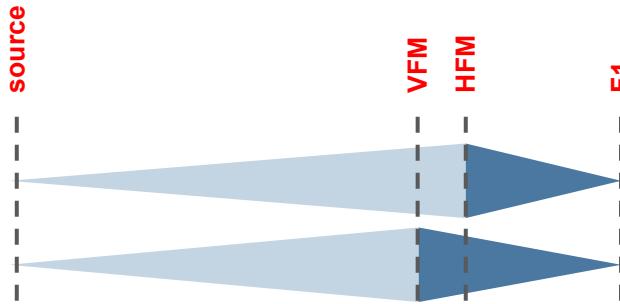
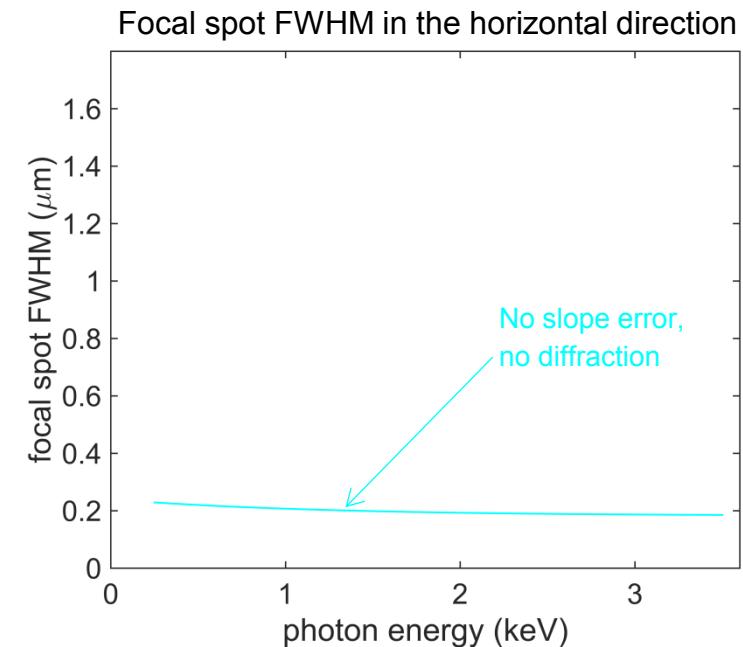
```
R-space
FkHx [mm], theta_fwm [urad]: 2.89758221191 3.11702045171
FkHy [mm], theta_fwm [urad]: 3.552090757523 3.8210959286
```



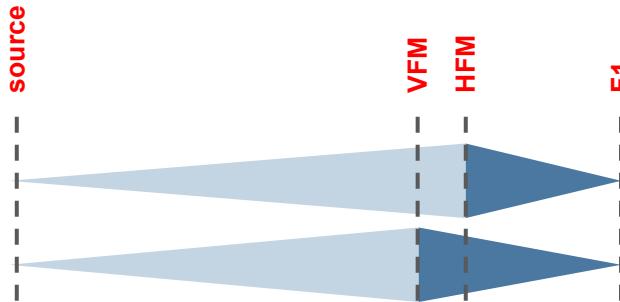
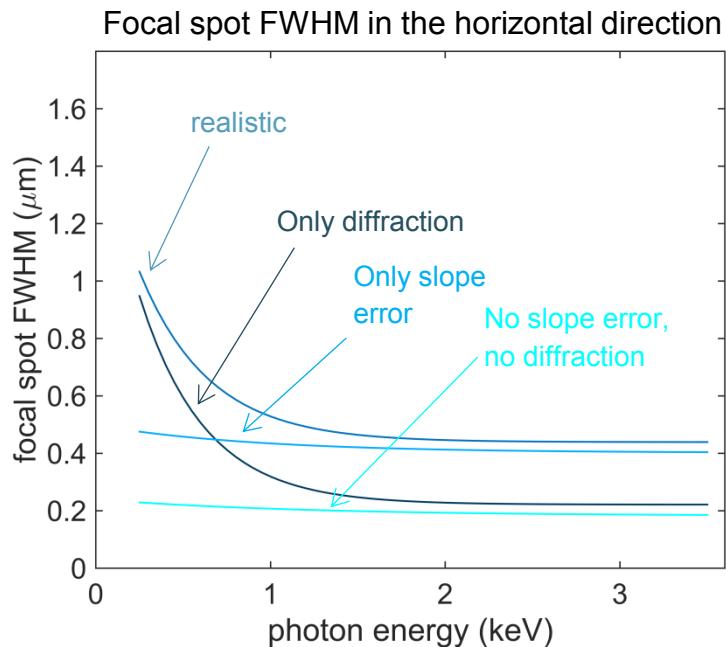
Propagating through BL2 beamline. Focused beam: perfect KB

```
print("*****Focused beam: perfect KB")
```

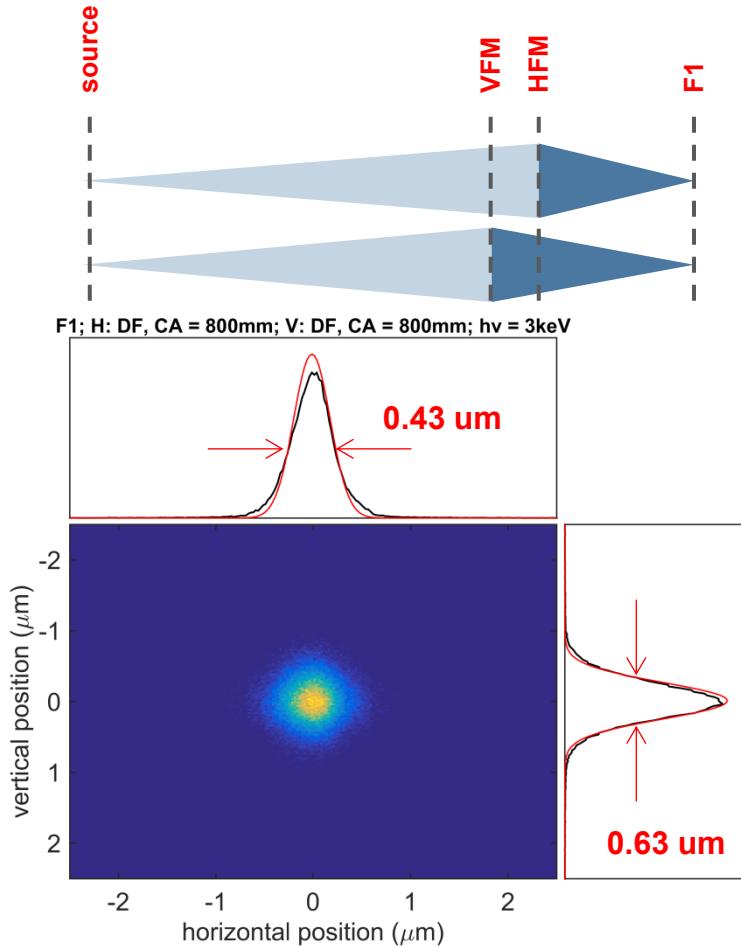
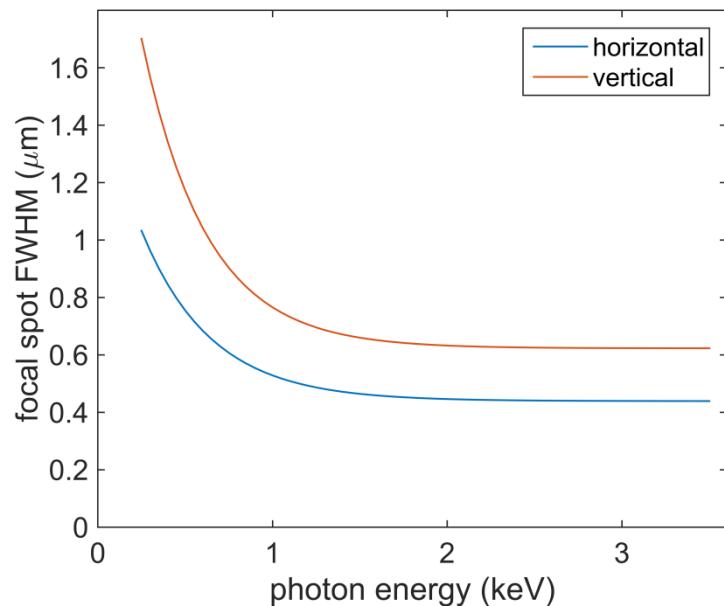
Ray tracing: Focusing performances in F1



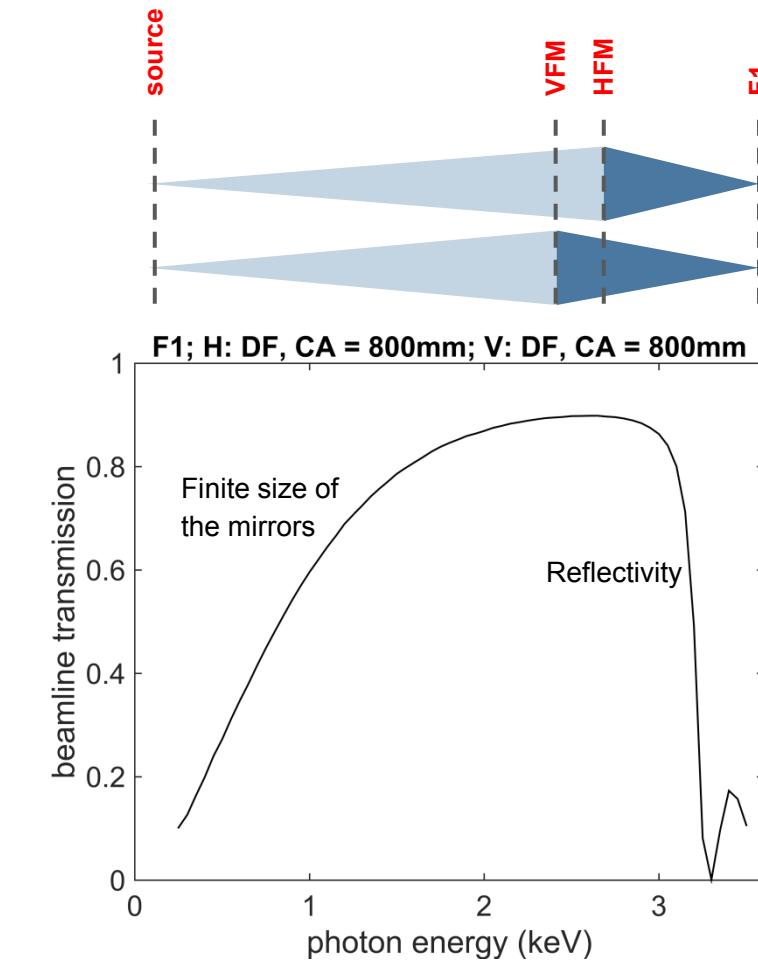
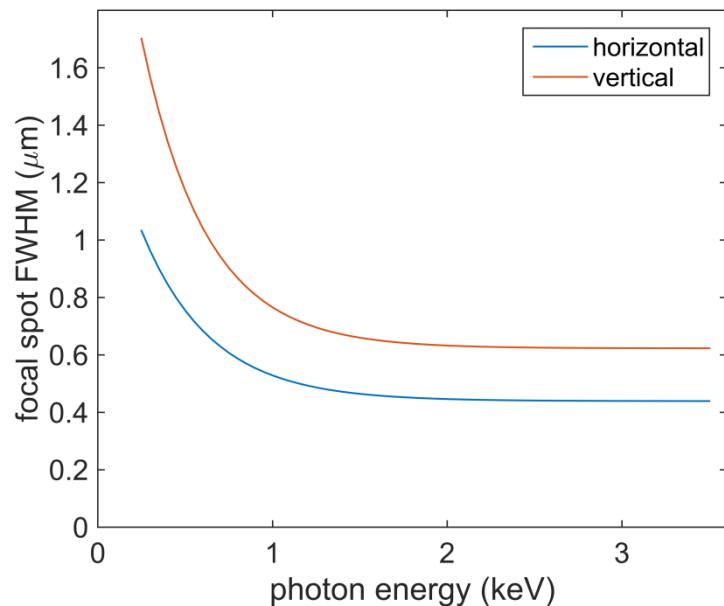
Ray tracing: Focusing performances in F1



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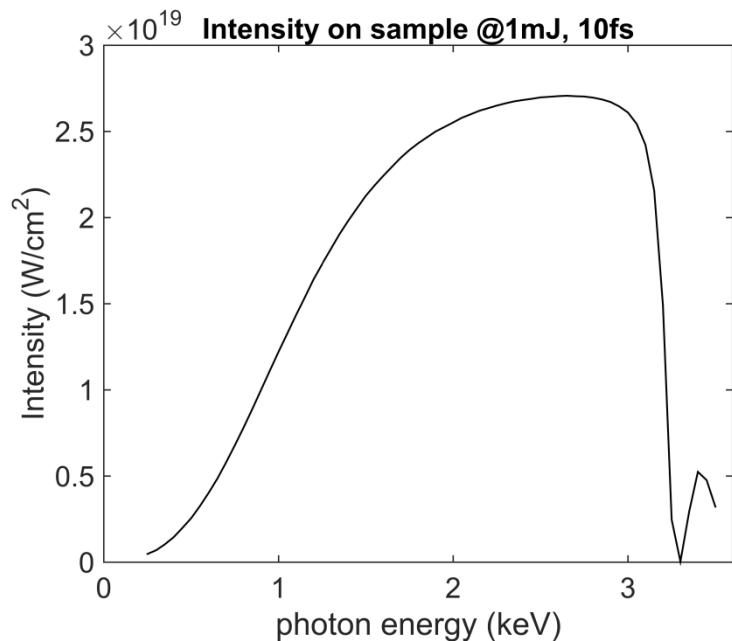


Ray tracing: Focusing performances in F1



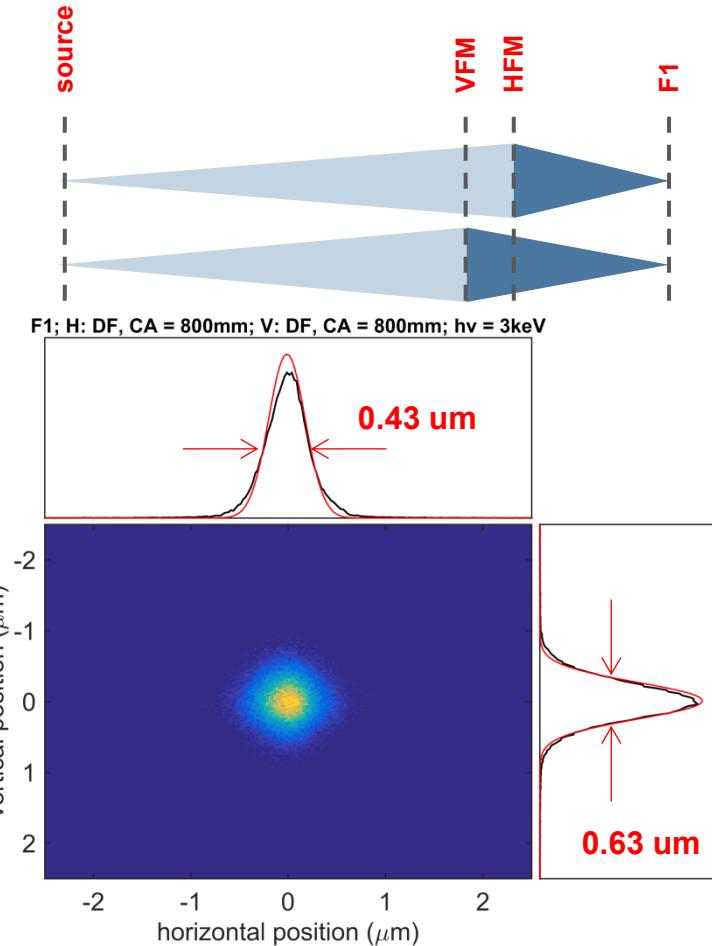
hv [keV]	Spot size FWHM [μm]	Transmission [%]
0,3	1,25	12
1	0,65	60
3	0,53	87

Ray tracing: Focusing performances in F1



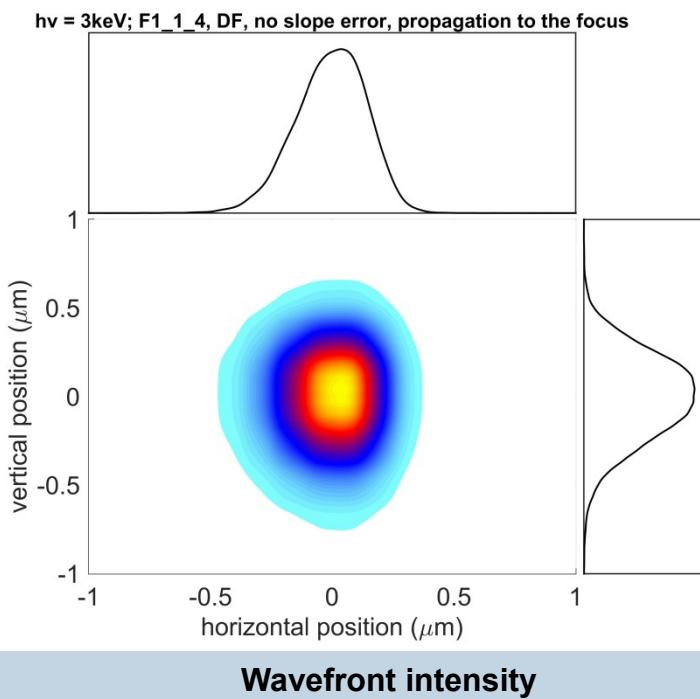
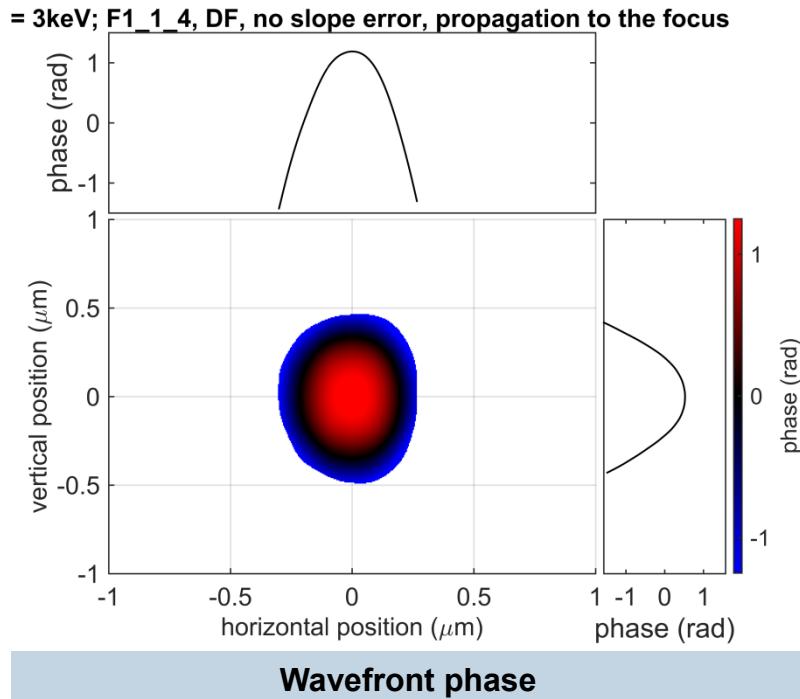
$$I = 8 \left(\frac{\log 2}{\pi} \right)^{3/2} E_p \cdot T_{beamline} \cdot \frac{1}{\tau \cdot FWHM^2}$$

European XFEL



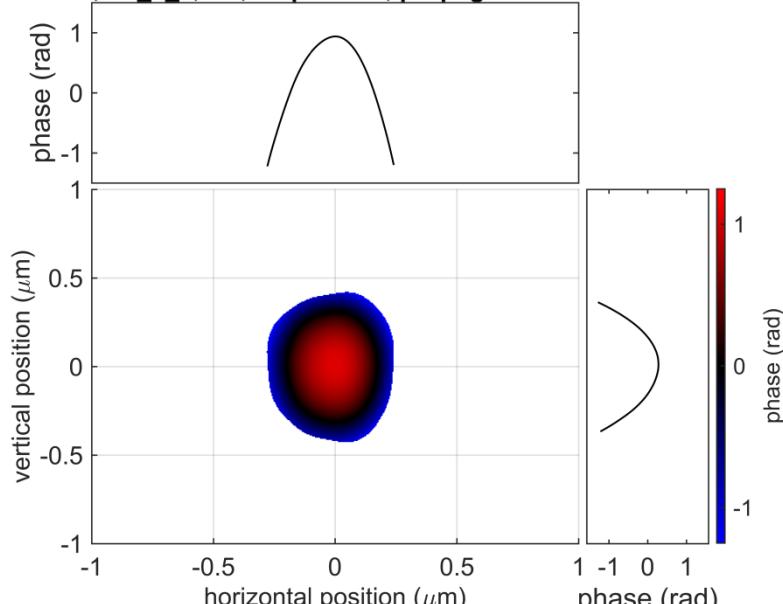
$h\nu$ [keV]	Spot size FWHM [μm]	Transmission [%]	Intensity [W/cm^2]
0,3	1,25	12	$7,0 \cdot 10^{17}$
1	0,65	60	$1,2 \cdot 10^{19}$
3	0,53	87	$2,6 \cdot 10^{19}$

Wavefront propagation: Wavefront in F1, $h\nu = 3 \text{ keV}$, without slope error



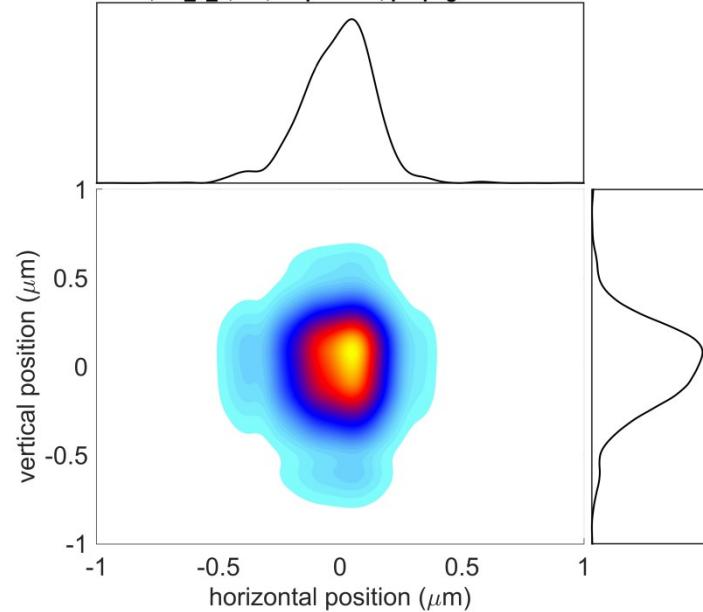
Wavefront propagation: Wavefront in F1, $h\nu = 3 \text{ keV}$, with slope error

$v = 3\text{keV}; F1_1_4, DF, \text{slope error, propagation to the focus}$



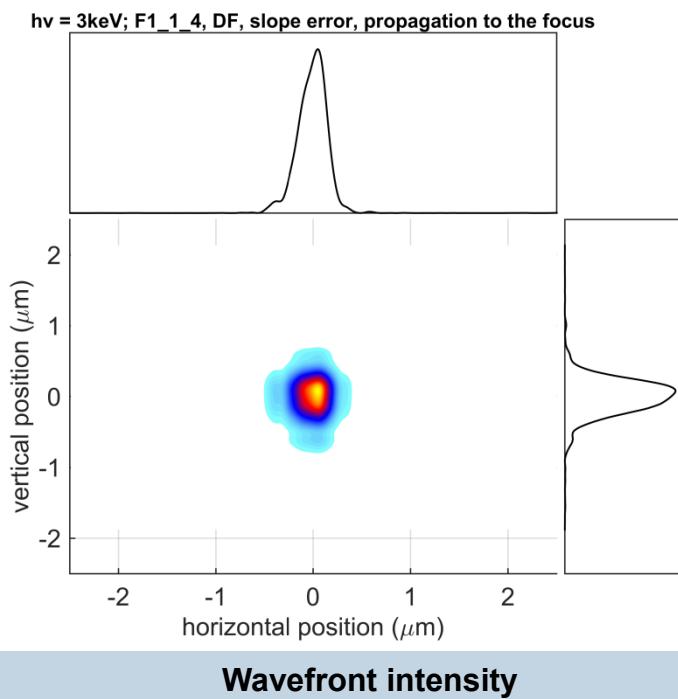
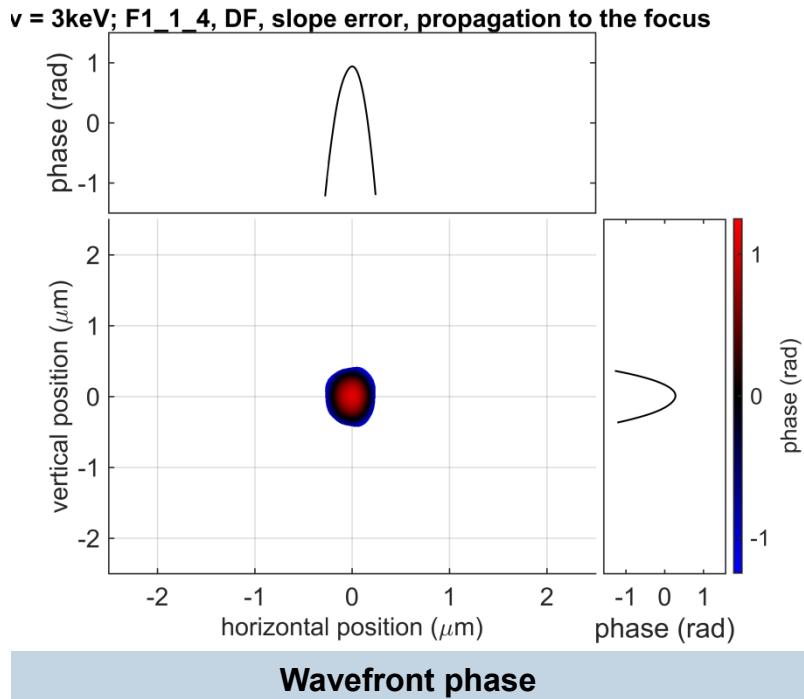
Wavefront phase

$h\nu = 3\text{keV}; F1_1_4, DF, \text{slope error, propagation to the focus}$



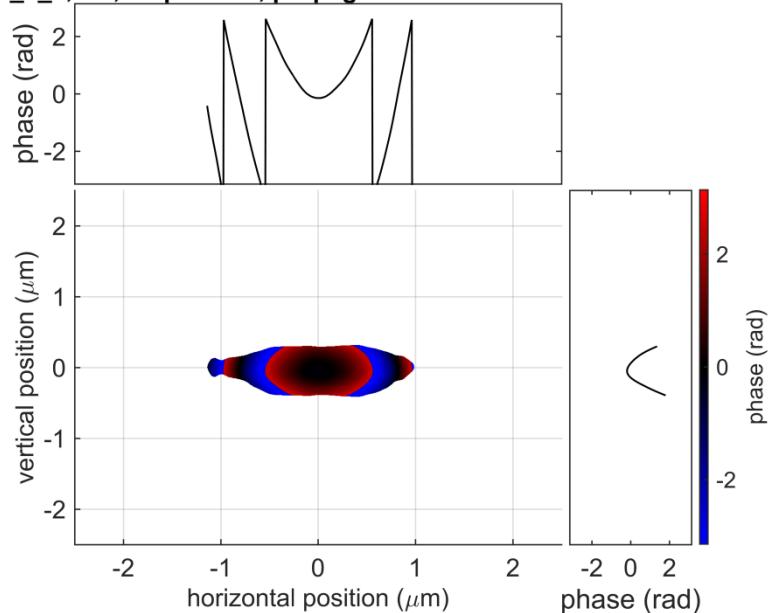
Wavefront intensity

Wavefront propagation: Wavefront in F1, $h\nu = 3 \text{ keV}$, with slope error



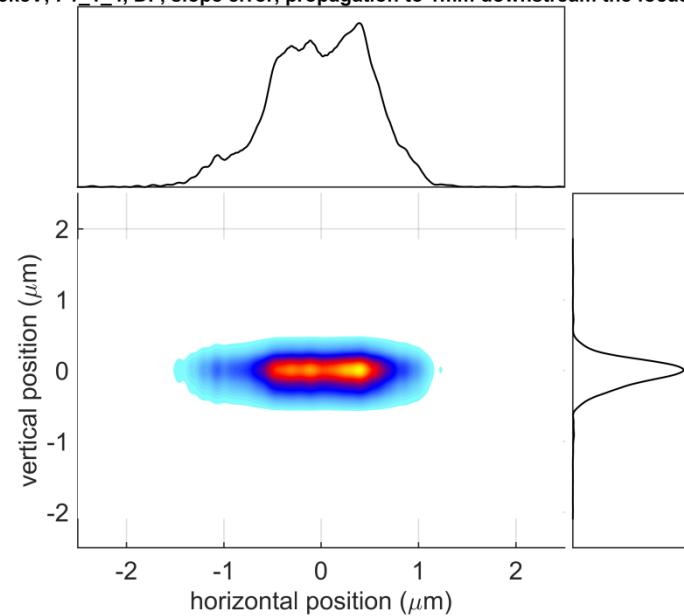
Wavefront in F1, $h\nu = 3 \text{ keV}$, with slope error, 1mm out of focus

F1_1_4, DF, slope error, propagation to 1mm downstream the focus



Wavefront phase

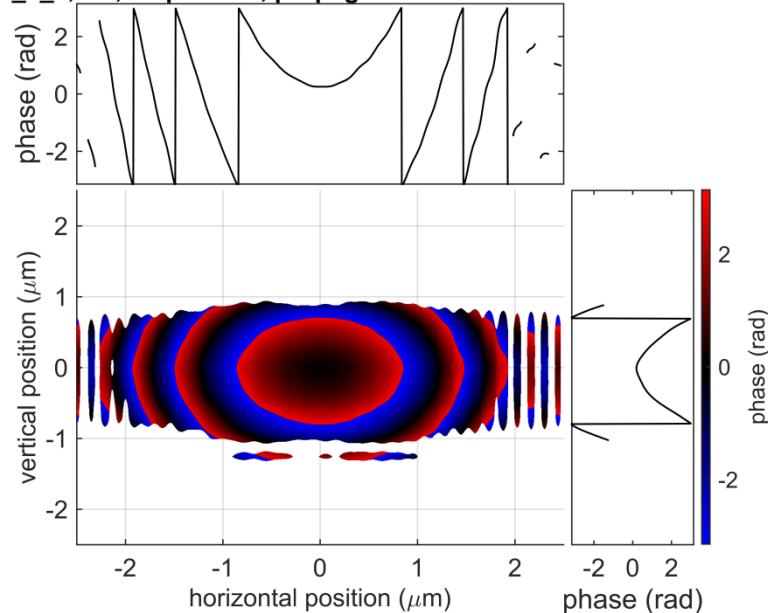
= 3keV; F1_1_4, DF, slope error, propagation to 1mm downstream the focus



Wavefront intensity

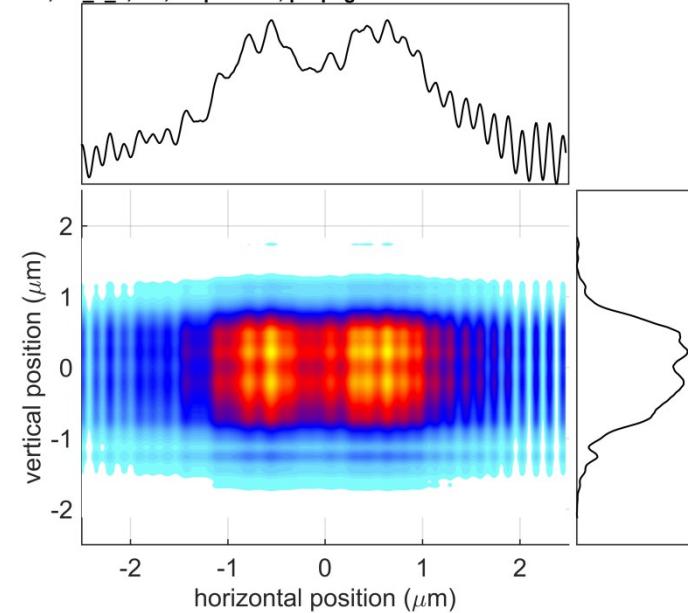
Wavefront in F1, $h\nu = 3 \text{ keV}$, with slope error, 2mm out of focus

F1_1_4, DF, slope error, propagation to 2mm downstream the focus



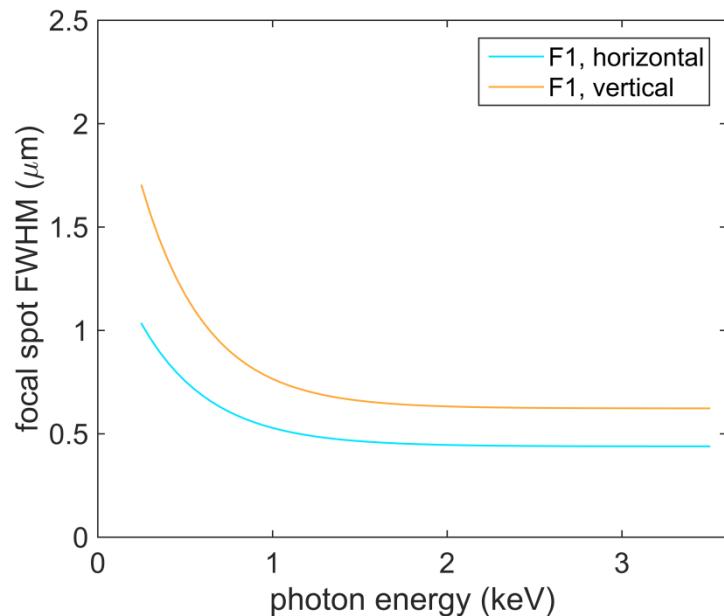
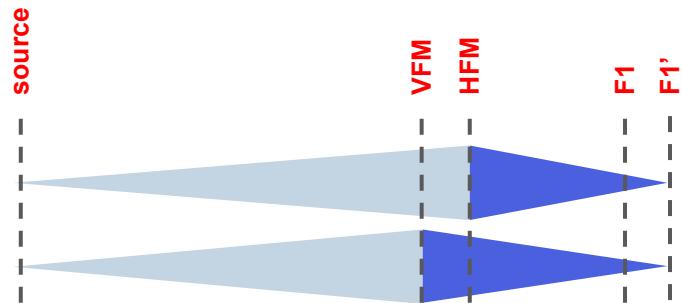
Wavefront phase

= 3keV; F1_1_4, DF, slope error, propagation to 2mm downstream the focus

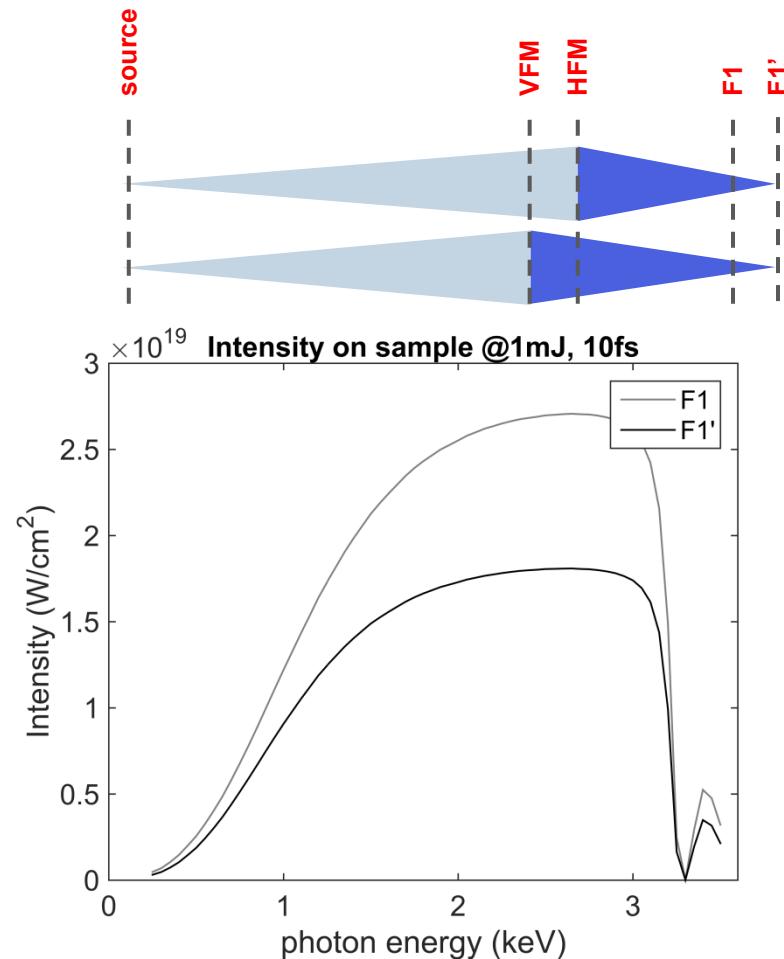
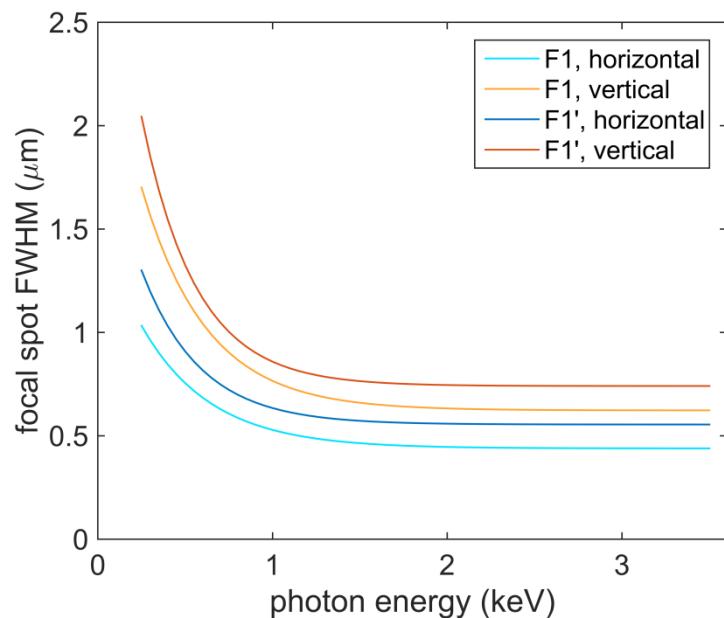


Wavefront intensity

Ray tracing: Focusing performances in F1'



Ray tracing: Focusing performances in F1'

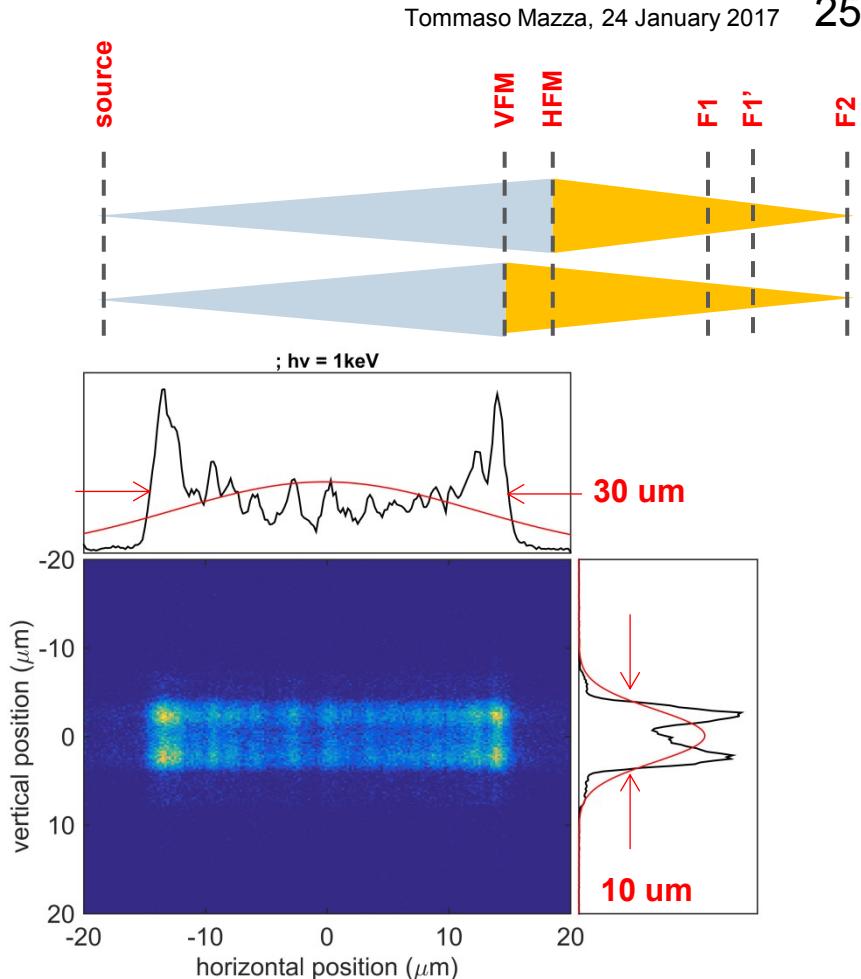


hv [keV]	Spot size FWHM [μm]	Transmission [%]	Intensity [W/cm ²]
0,3	1,52	12	$4,7 \cdot 10^{17}$
1	0,75	60	$9,0 \cdot 10^{18}$
3	0,65	87	$1,7 \cdot 10^{19}$

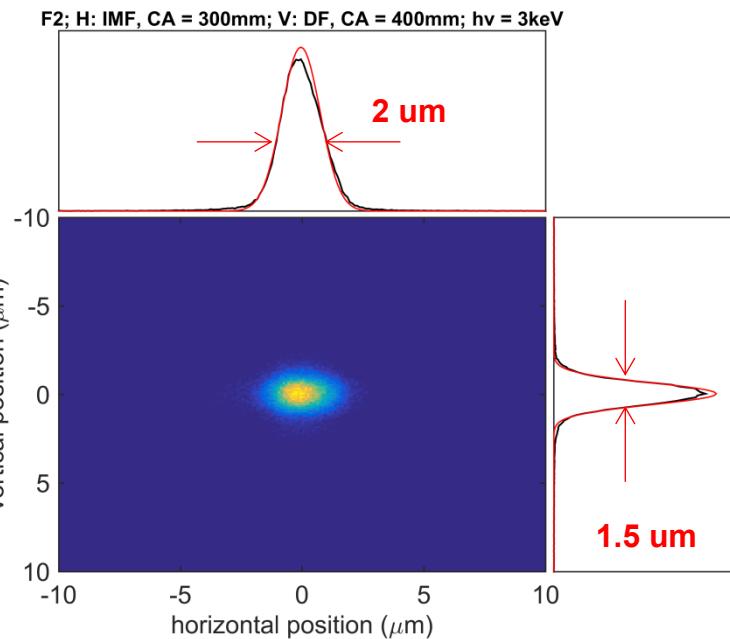
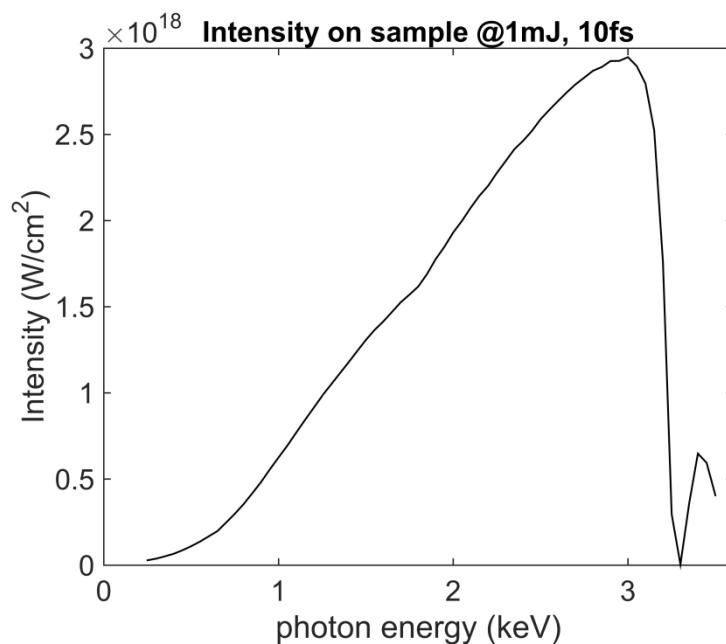
Ray tracing:

Focusing performances in F2

KB	focus	p [m]	q [mm]	Clear aperture [mm]	Error [nrad RMS]
HFM	F1	433,9	1800	800	0
VFM	F1	432,7	3000	800	0
HFM	F1'	433,9	2150	800	15
VFM	F1'	432,7	3350	800	9
HFM	F2	433,9	3832	800	1652
VFM	F2	432,7	5032	800	280



Focusing performances in F2 – what is in fact possible (in the way described in the next slides)



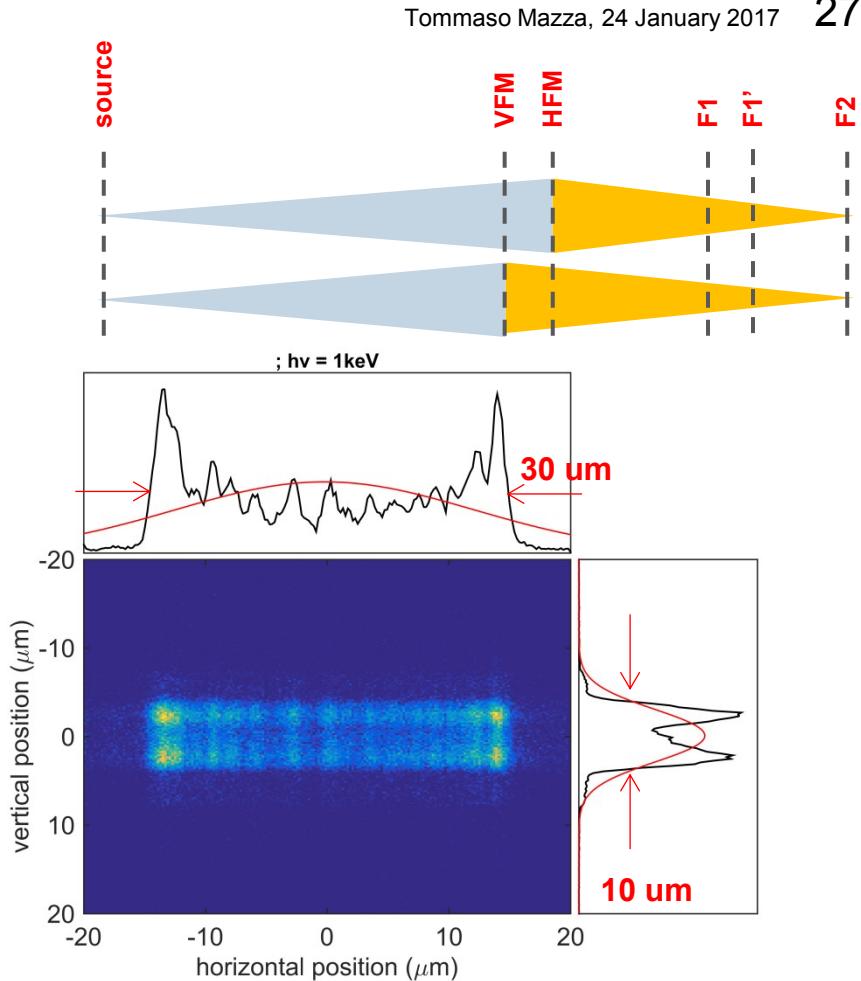
$h\nu$ [keV]	Spot size FWHM* [μm]	Intensity* [W/cm^2]
0,3	5,1	$3,8 \cdot 10^{16}$
1	2,1	$6,3 \cdot 10^{17}$
3	1,7	$2,9 \cdot 10^{18}$

(*): not matching each other

Ray tracing:

Focusing performances in F2

KB	focus	p [m]	q [mm]	Clear aperture [mm]	Error [nrad RMS]
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VFM	F1	432,7	3000	800	0
HFM	F1'	433,9	2150	800	15
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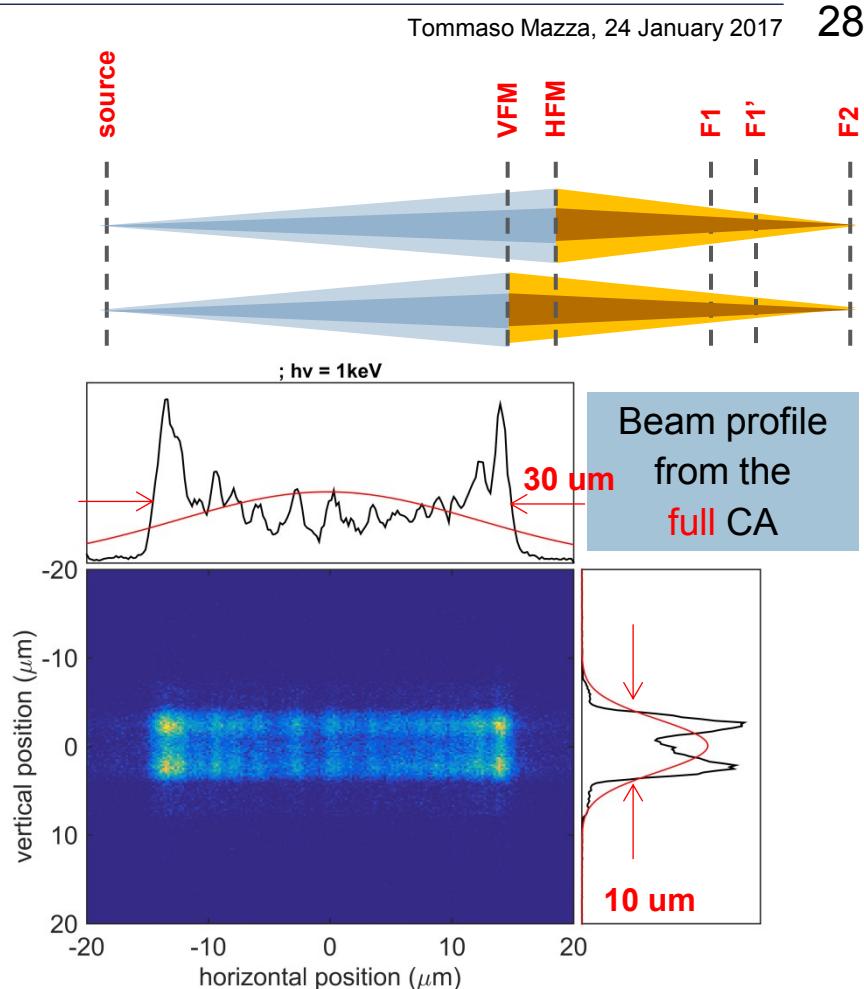
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HFM	F2	433,9	3832	800	1652
VFM	F2	432,7	5032	800	280
HFM	F2	433,9	3832	400	264
VFM	F2	432,7	5032	600	118

Handles:

- Slit down the beam



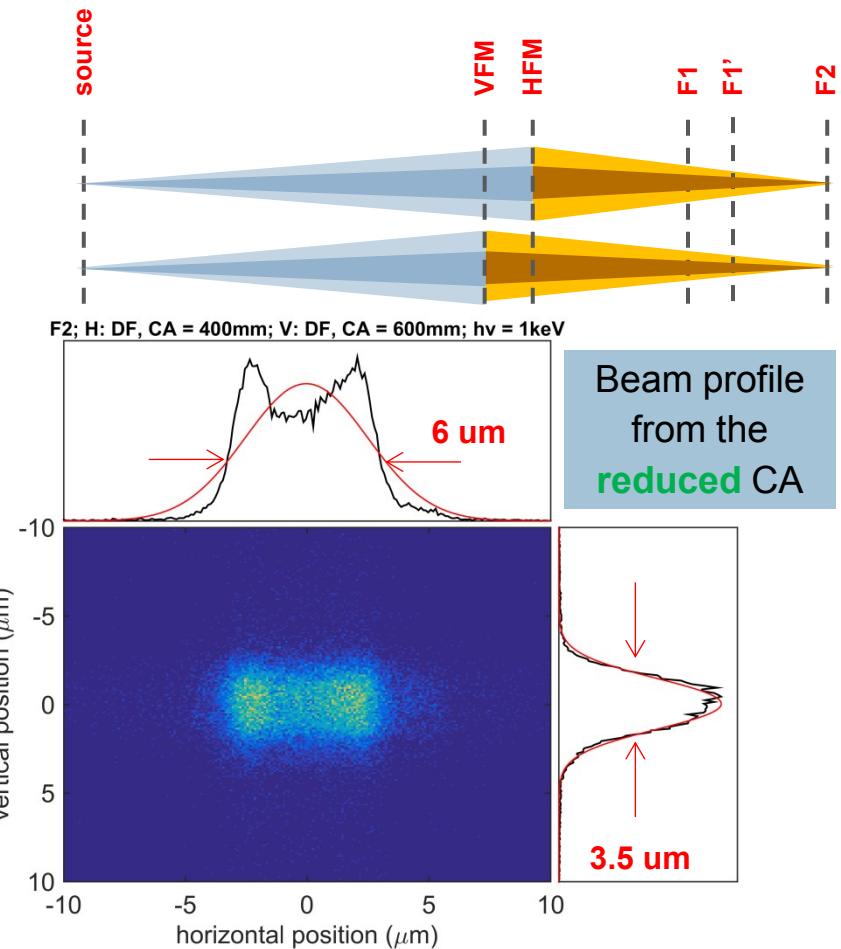
The bending couples are optimized on the reduced clear aperture

Ray tracing: Focusing performances in F2

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HFM	F2	433,9	3832	400	264
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Handles:

- Slit down the beam



The bending couples are optimized on the reduced clear aperture

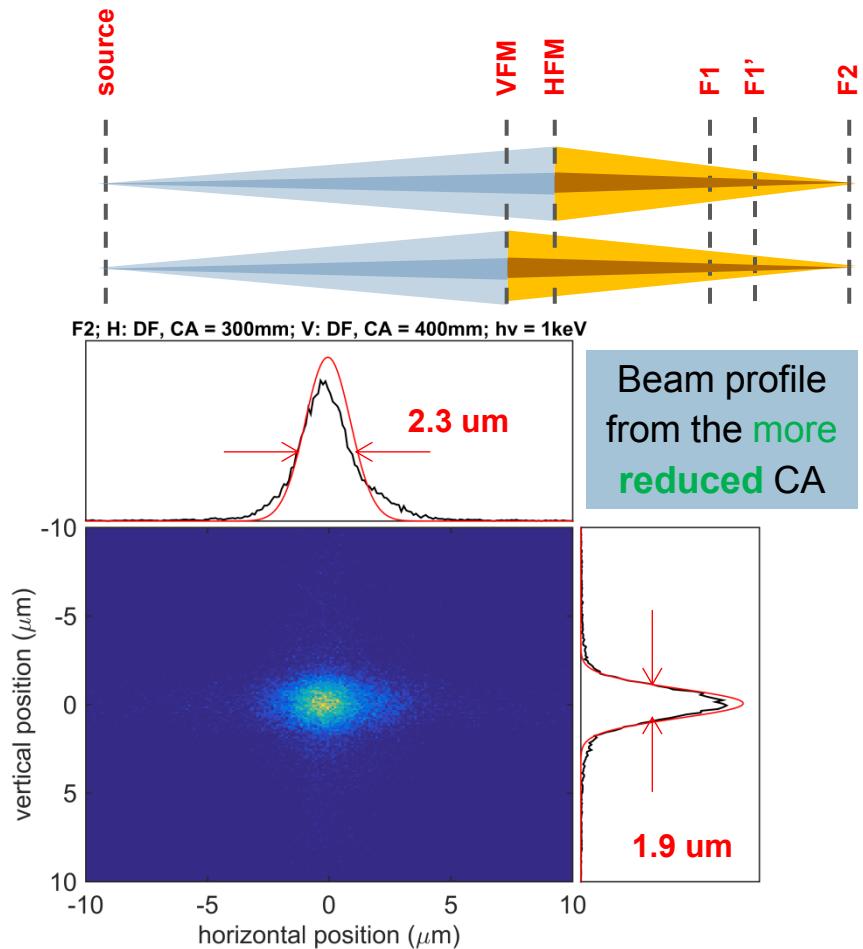
Ray tracing:

Focusing performances in F2

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HFM	F1'	433,9	2150	800	15
VFM	F1'	432,7	3350	800	9
HFM	F2	433,9	3832	800	1652
VFM	F2	432,7	5032	800	280
HFM	F2	433,9	3832	300	130
VFM	F2	432,7	5032	400	40

Handles:

- Slit down the beam



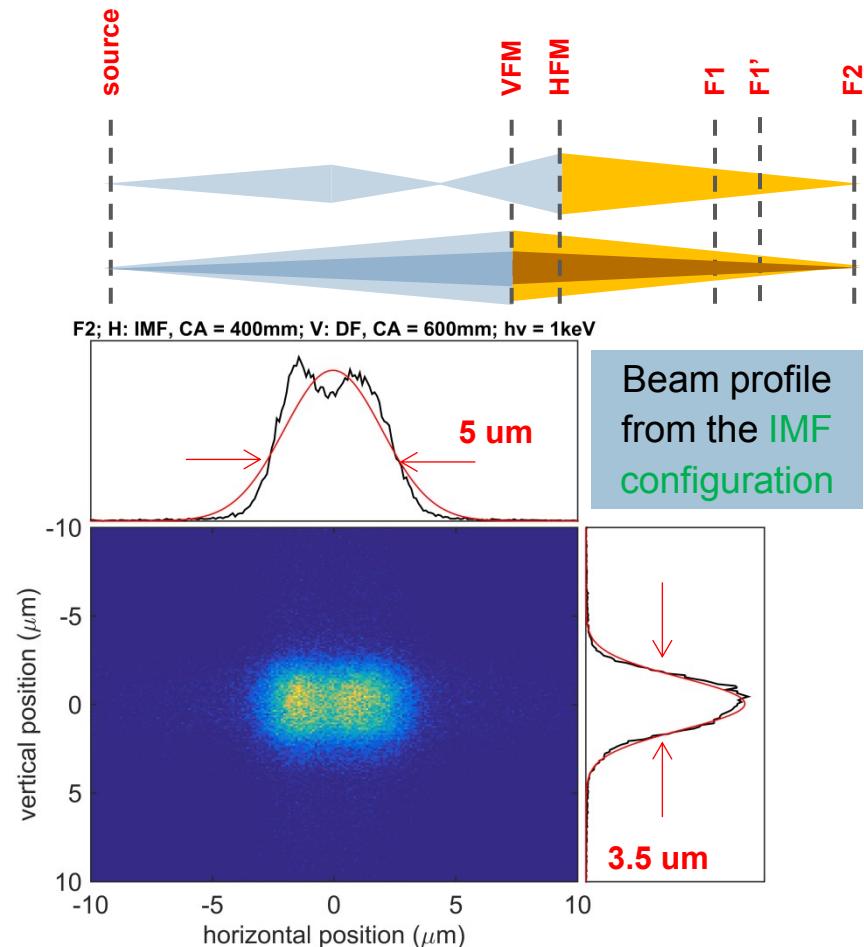
The bending couples are optimized on the reduced clear aperture

Ray tracing: Focusing performances in F2

KB	focus	p [m]	q [mm]	Clear aperture [mm]	Error [nrad RMS]
HFM	F1	433,9	1800	800	0
VFM	F1	432,7	3000	800	0
HFM	F1'	433,9	2150	800	15
VFM	F1'	432,7	3350	800	9
HFM	F2	433,9	3832	800	1652
VFM	F2	432,7	5032	800	280
HFM	F2	72	3832	400	185
VFM	F2	432,7	5032	600	118

Handles:

- Slit down the beam
- Use the H intermediate focus



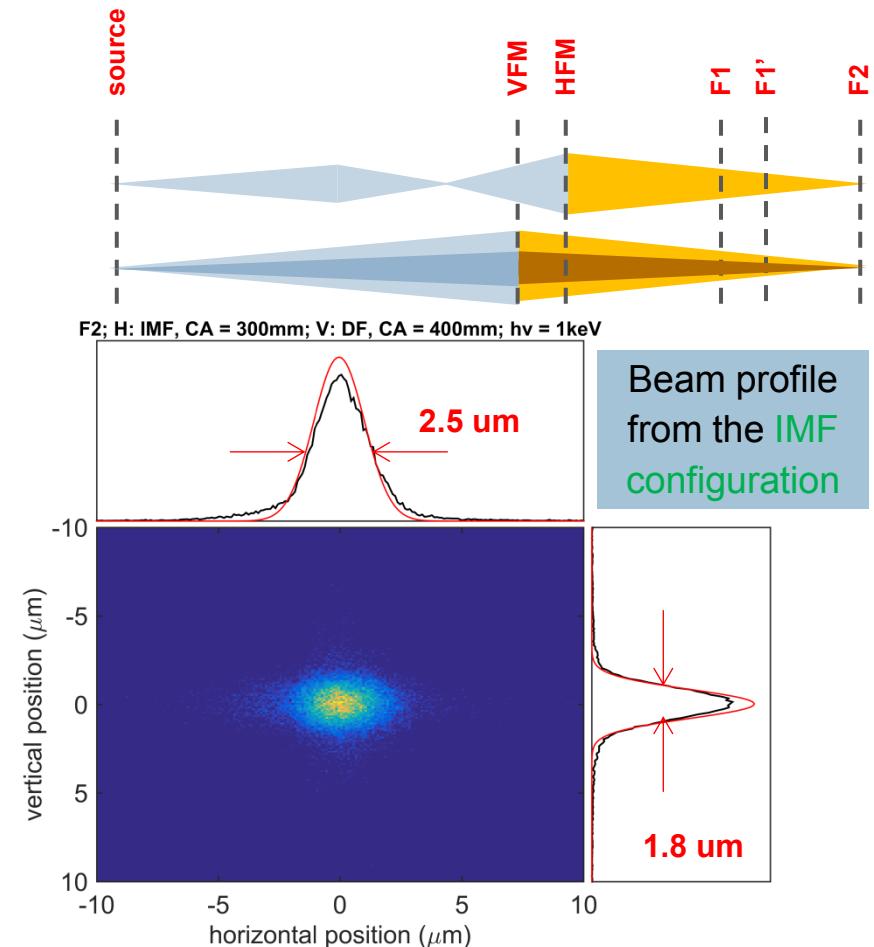
Ray tracing:

Focusing performances in F2

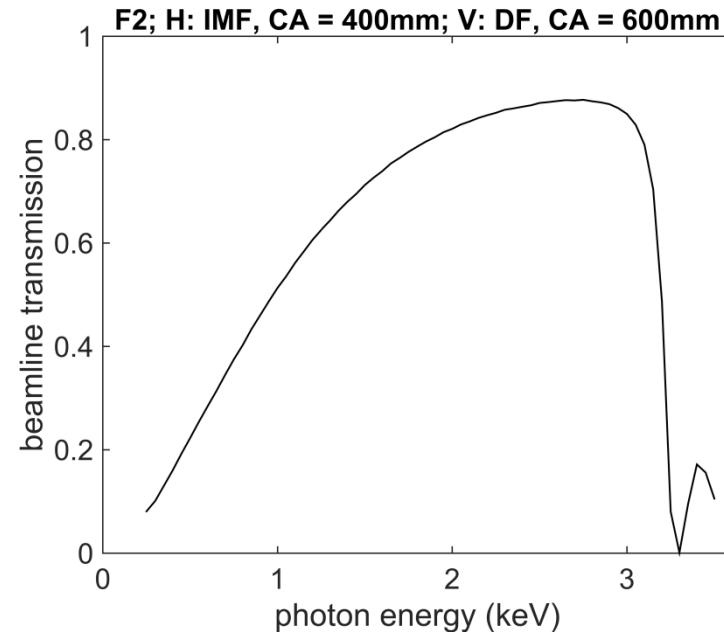
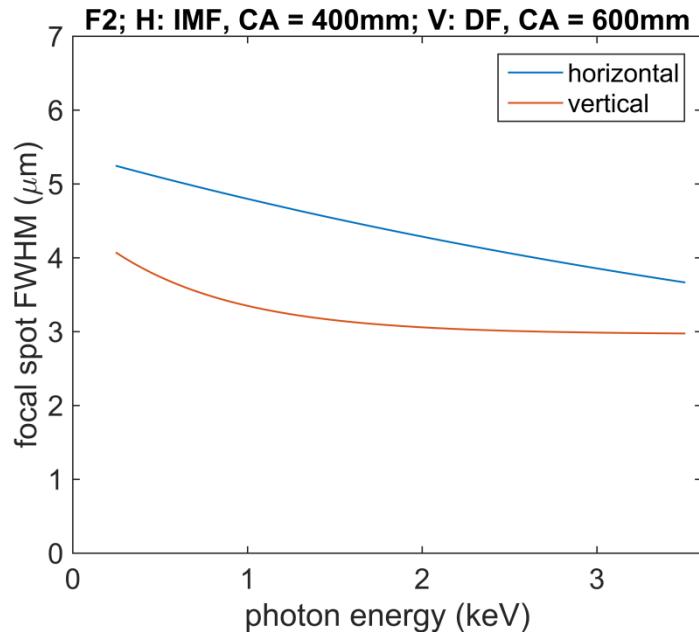
KB	focus	p [m]	q [mm]	Clear aperture [mm]	Error [nrad RMS]
HFM	F1	433,9	1800	800	0
VFM	F1	432,7	3000	800	0
HFM	F1'	433,9	2150	800	15
VFM	F1'	432,7	3350	800	9
HFM	F2	433,9	3832	800	1652
VFM	F2	432,7	5032	800	280
HFM	F2	72	3832	300	131
VFM	F2	432,7	5032	400	40

Handles:

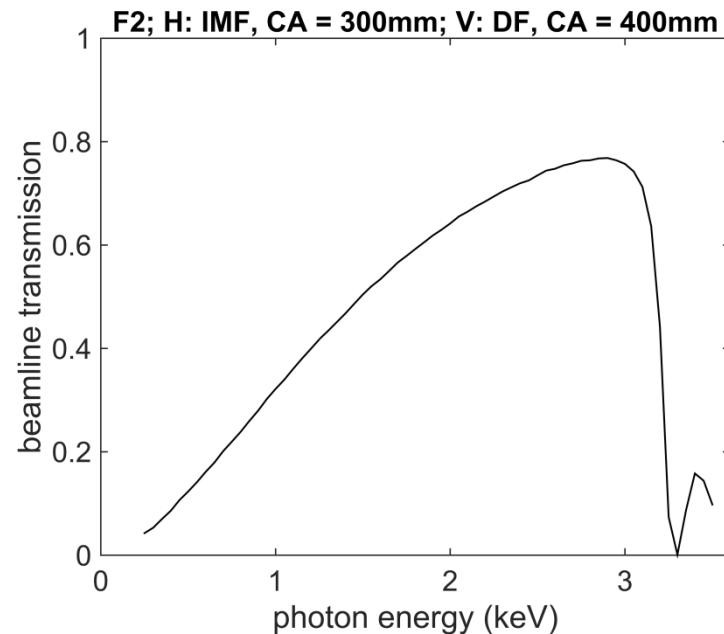
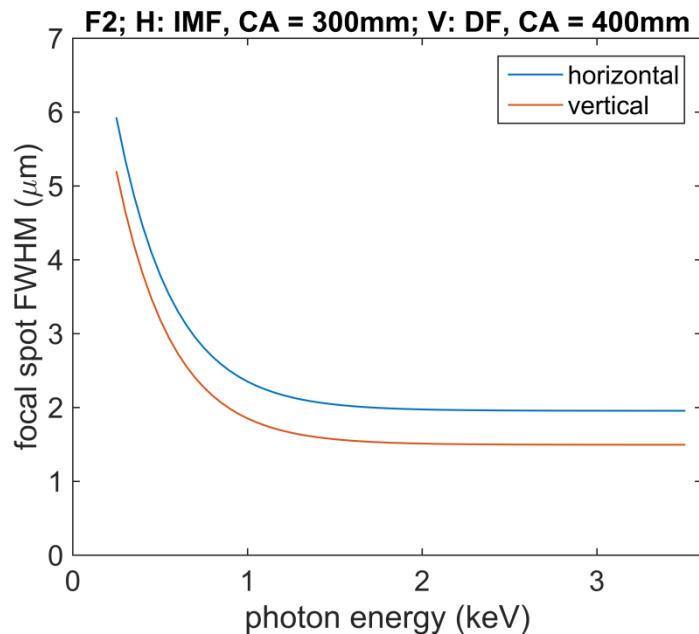
- Slit down the beam
- Use the H intermediate focus



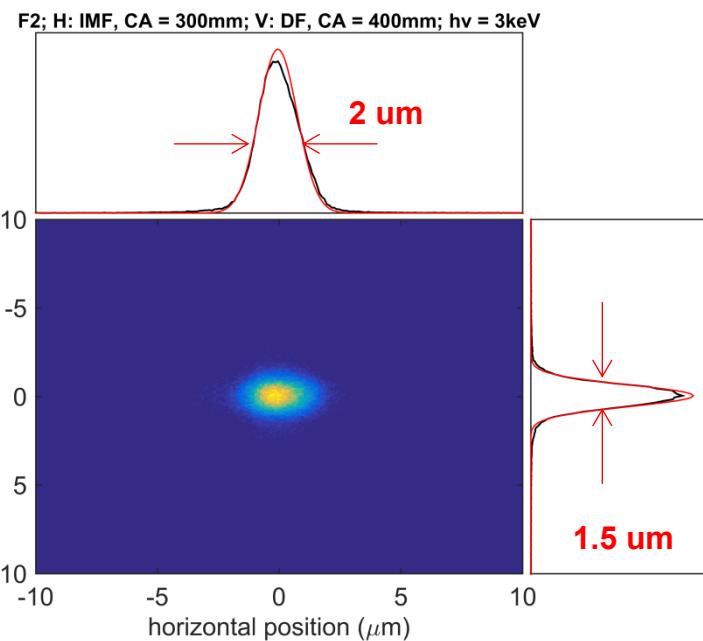
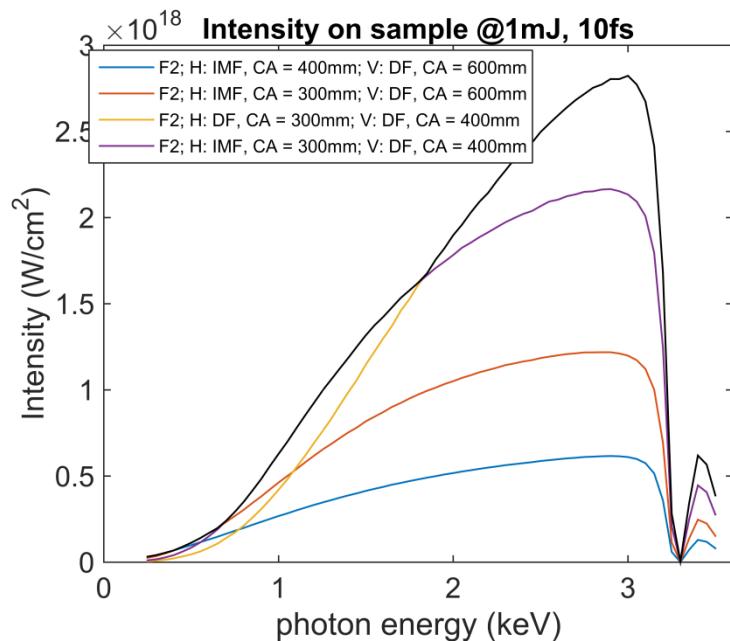
Ray tracing: Focusing performances in F2: H IMF, CA=400; V DF, CA=600



Ray tracing: Focusing performances in F2: H IMF, CA=300; V DF, CA=400



Ray tracing: Focusing performances in F2

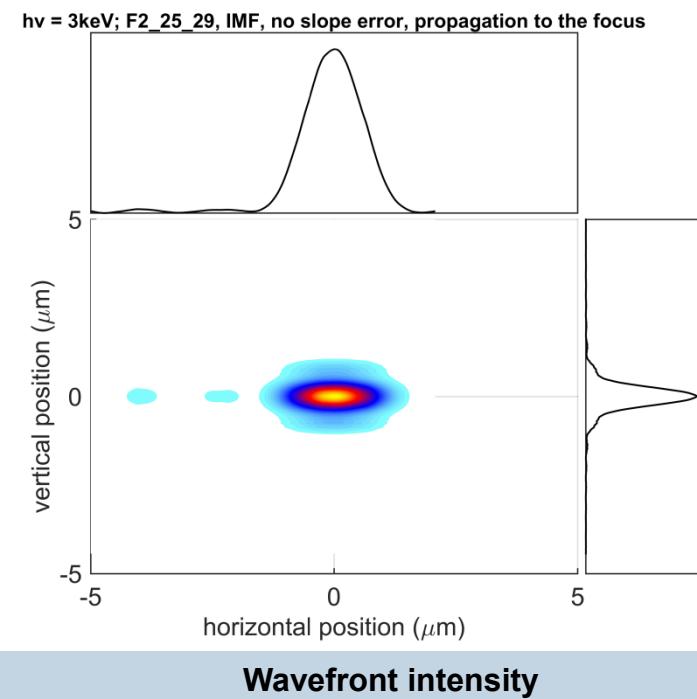
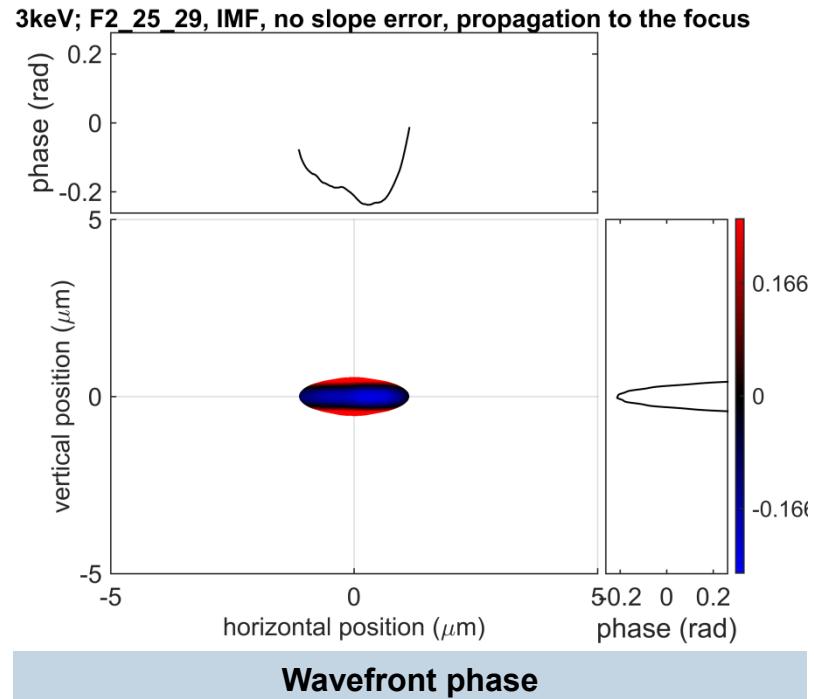


European XFEL

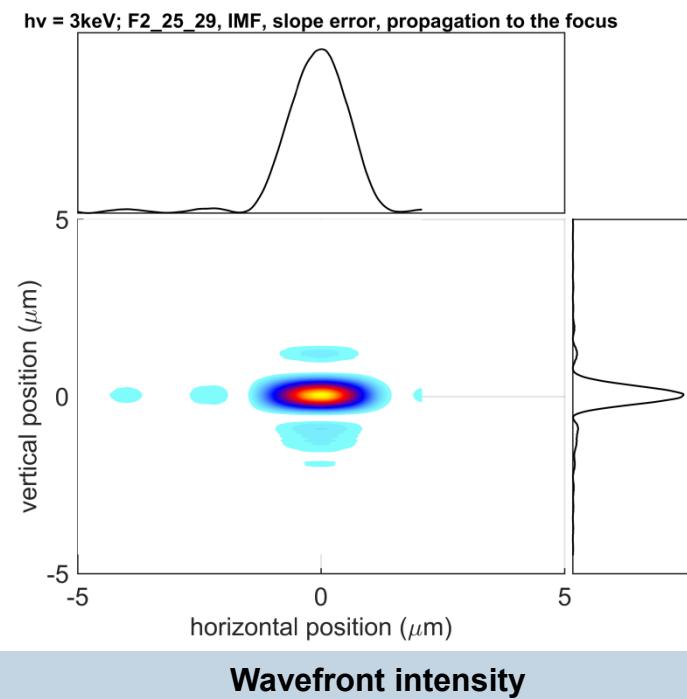
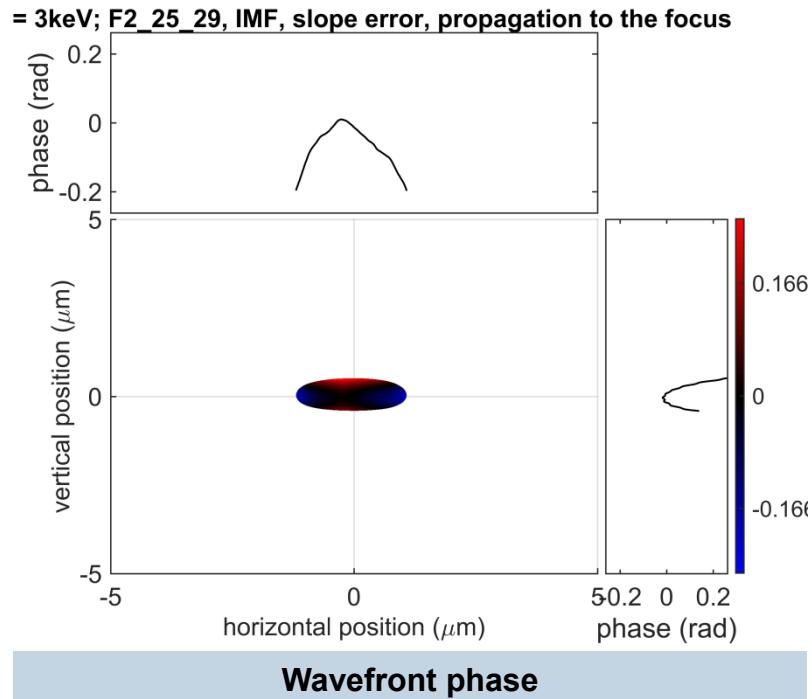
hν [keV]	Spot size FWHM* [μm]	Intensity* [W/cm²]
0,3	5,1	$3,8 \cdot 10^{16}$
1	2,1	$6,3 \cdot 10^{17}$
3	1,7	$2,9 \cdot 10^{18}$

(*): not matching each other

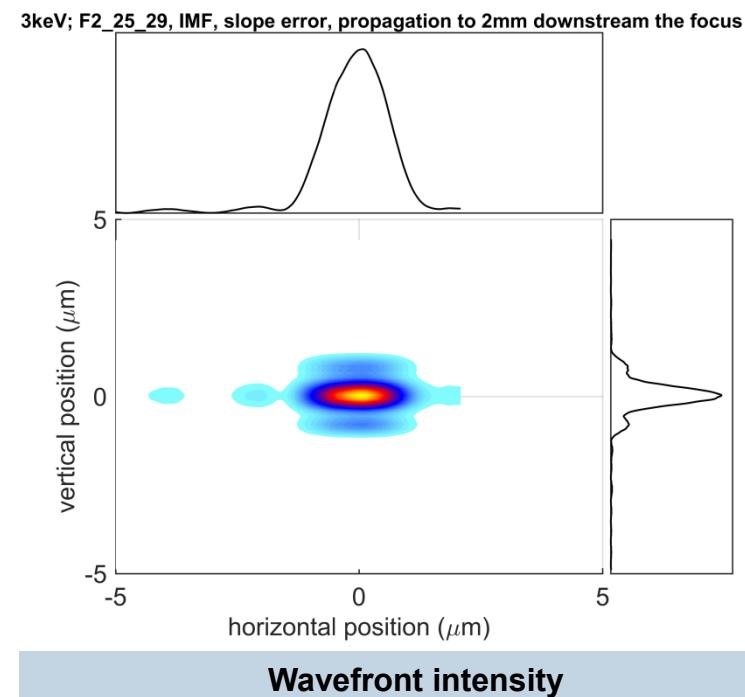
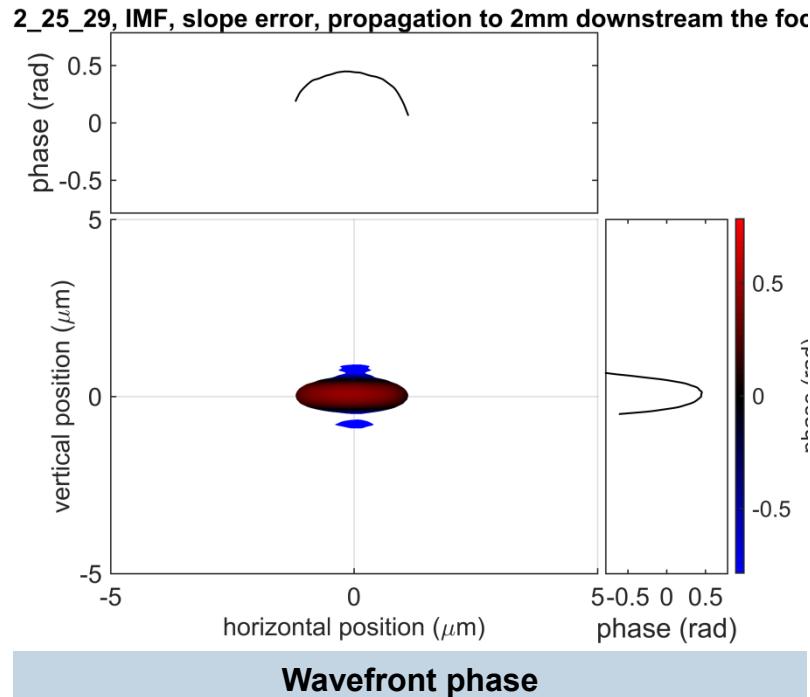
Wavefront in F2 – H IMF, CA=300; V DF, CA=400, w/o sl. err $h\nu = 3\text{keV}$, in focus



Wavefront in F2 – H IMF, CA=300; V DF, CA=400, with sl. err $h\nu = 3\text{keV}$, in focus



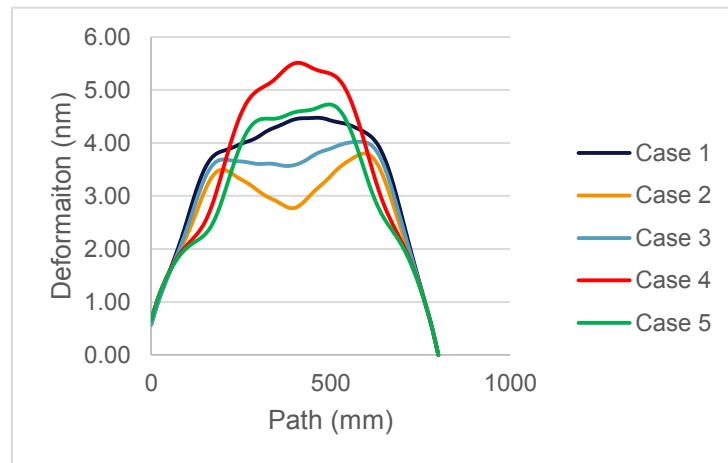
Wavefront in F2 – H IMF, CA=300; V DF, CA=400, with sl. err $h\nu = 3\text{keV}$, 2mm out of focus



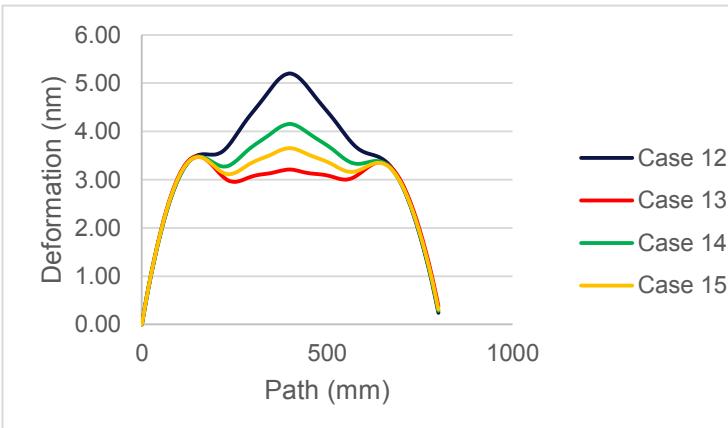
The effect of the thermal load

- Thermal load from FEL radiation induces surface modification on the nanometer level
- The effect can be quantified by finite element analysis; FEA can be used to optimize the cooling grooves geometry
- The deformation corresponding to the optimal cooling arrangement can be fed to the ray tracing simulations to obtain expected performances

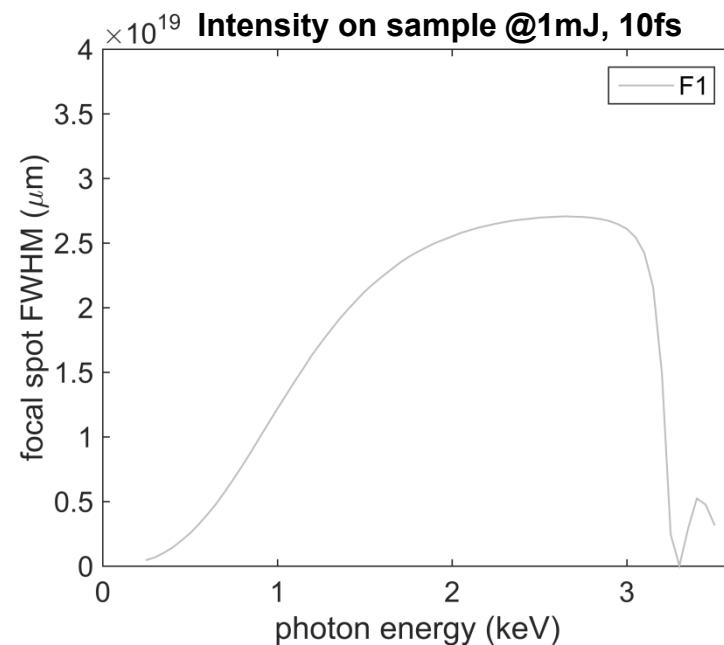
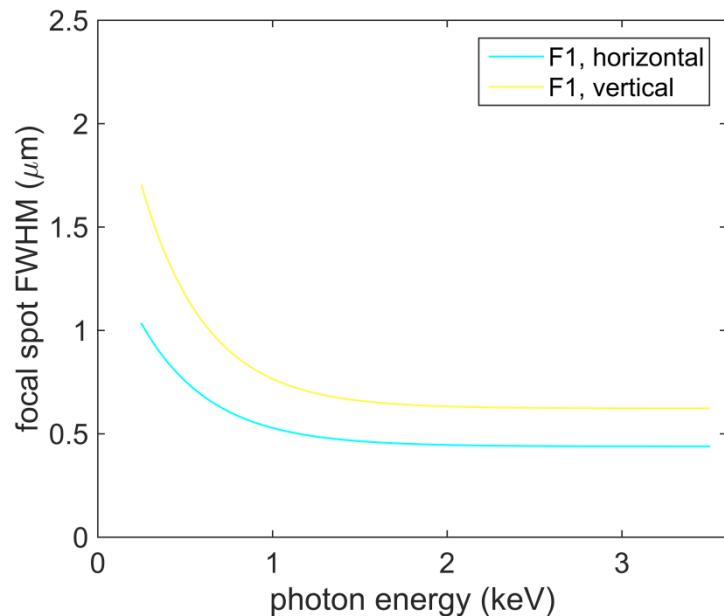
VFM Thermal deformation under “standard” conditions



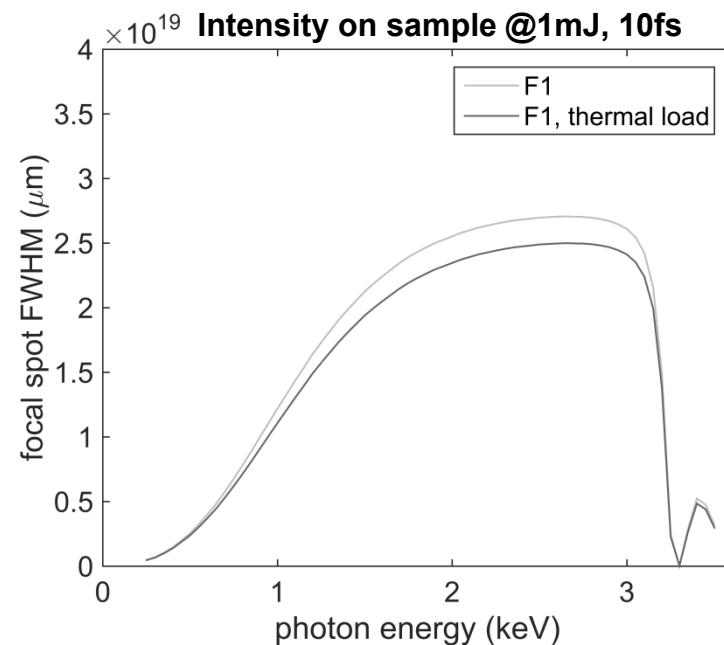
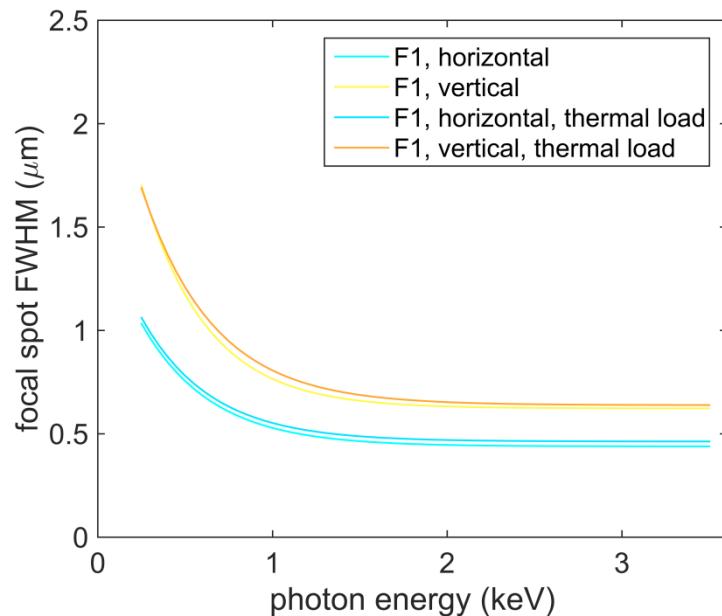
HFM Thermal deformation under “standard” conditions



Ray tracing: Focusing performances in F1 including thermal load



Ray tracing: Focusing performances in F1 including thermal load



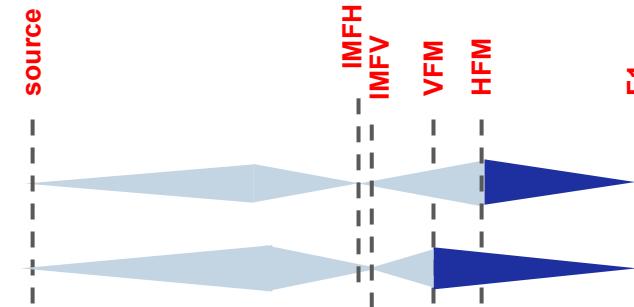
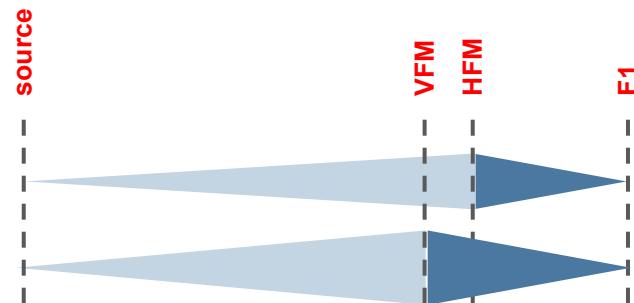
Possible interim solution for instrument commissioning and 1st experiment

- Expected delivery of the SQS mirrors:
December 2017 (+ metrology + coating + ...)
- Plan to be ready from commissioning activities:
End of 2017

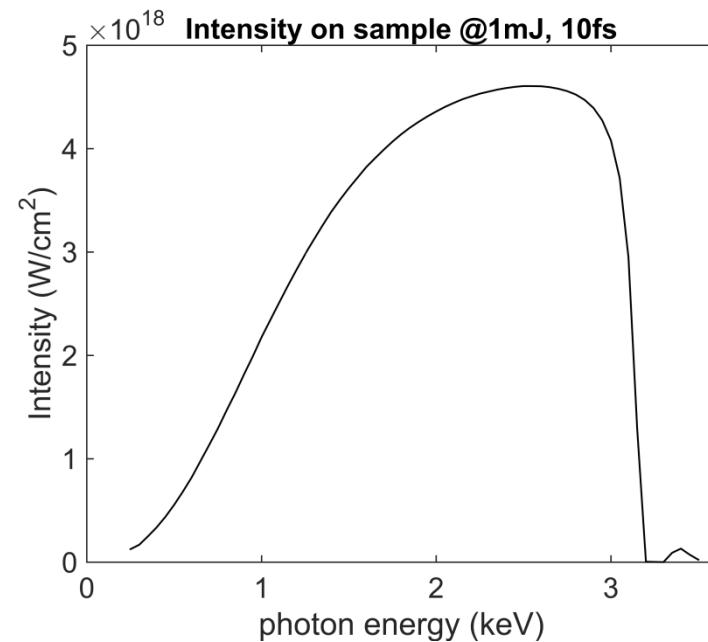
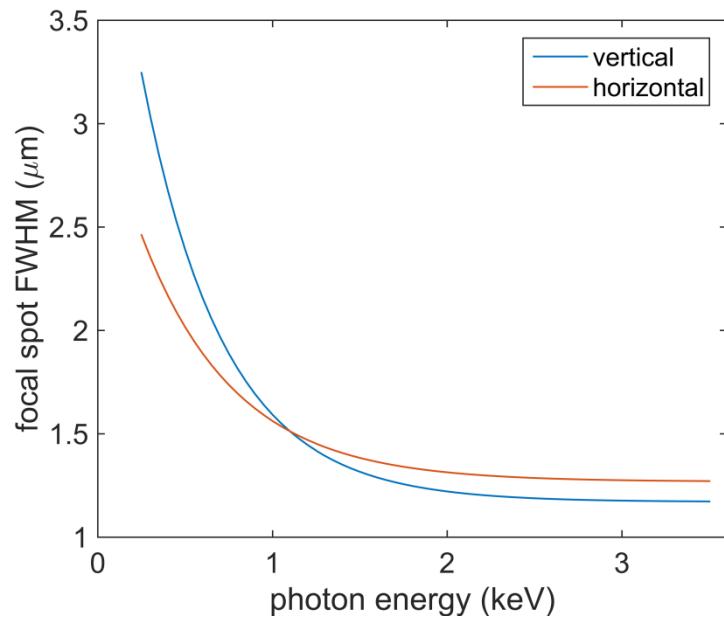
■ Possible interim solution:

Mis-cut SCS/SQS non-bendable mirrors, to be adapted to the SQS beamline layout by incidence angle detuning

- Parameters (H): $p = 52\text{m}$; $q = 3.3\text{m}$; $\theta = 9\text{mrad}$
 - ▶ $p = 71\text{m}$; $q = 3.3\text{m} \rightarrow \theta = 9.14\text{mrad}$
- Parameters (V): $p = 28\text{m}$; $q = 2.0\text{m}$; $\theta = 9\text{mrad}$
 - ▶ $p = 43\text{m}$; $q = 2.0\text{m} \rightarrow \theta = 9.24\text{mrad}$



Ray tracing: Interim solution expected performances



hv [keV]	Spot size FWHM [μm]	Transmission [%]	Intensity [W/cm²]
0,3	2,7	15	1,8 10¹⁷
1	1,6	65	2,1 10¹⁸
3	1,22	75	4,1 10¹⁸

Characterization methods

- wavefront sensor
- Imagine optic
- E. Ploenies, K. Tiedtke

- Knife edge characterization

- Pmma imprinting method

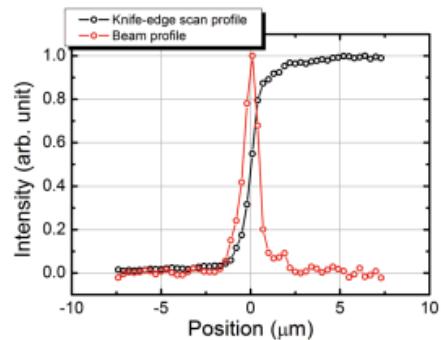
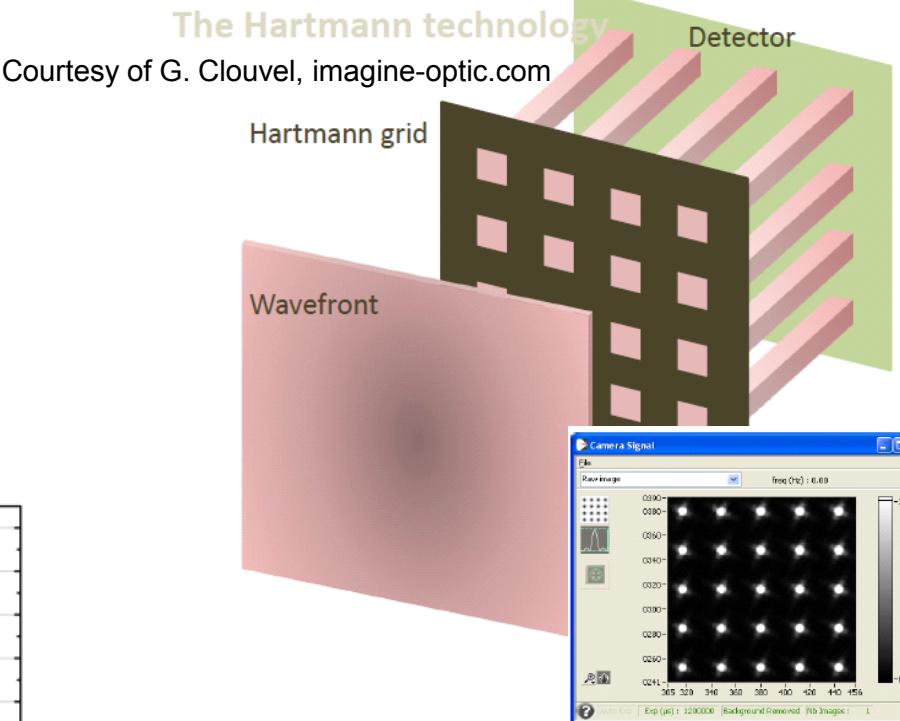


Figure 1. Typical beam profile measured with knife-edge scanning method in the horizontal direction.



Ishikawa et al., Journal of Physics: Conference Series 463 (2013) 012043

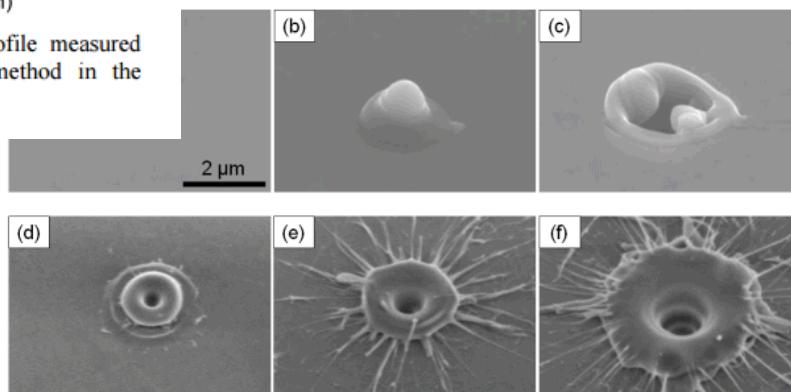


Figure 2. (a–c) Imprint SEM images of silicon under angle of 45° at fluence of $2.7 \mu\text{J}/\mu\text{m}^2$, $4.3 \mu\text{J}/\mu\text{m}^2$, and $6.7 \mu\text{J}/\mu\text{m}^2$. Imprint diameters were 1.1 μm, 2.4 μm, and 3.1 μm. (d–e) Imprint SEM images of synthetic fused silica under angle of 30° at fluence of $6.7 \mu\text{J}/\mu\text{m}^2$, $8.3 \mu\text{J}/\mu\text{m}^2$, and $12 \mu\text{J}/\mu\text{m}^2$. Imprint diameters were 1.7 μm, 2.4 μm, and 3.8 μm.

Summary

- Focusing system functional specifications coping with
 - Science case
 - Source, beamline, instrument characteristics
- Conceptual and technical solution for the SQS KB system
- Expected performances: results from simulations
 - ray tracing
 - wavefront propagation
- The solution for day one
- Characterization tools

- Adaptive elliptical pre-polished mirrors with mechanical benders and cooling system
- CDR specifications are met:
 - ray tracing:
 - ▶ Beam is nicely shaped in the focal spot; <1um (F1,F1'); <2um (F2) ($h\nu > 1\text{keV}$)
 - ▶ Intensity: $10^{17} - 10^{19} \text{ W/cm}^2$ (F1,F1'); $10^{16} - 10^{18} \text{ W/cm}^2$ (F2)
 - ▶ Thermal load effects are well compensated by the optimized cooling design
 - ▶ Acceptable focusing conditions from the day one solution
 - Wavefront propagation:
 - ▶ curved wavefront in F1 (and F1'), more flat in F2
 - ▶ Wavefront is not affected significantly by residual polishing and bending surface error
 - Elliptical mirrors with fixed profile, angle-detuned to adapt to the SQS beamline geometry
 - Different solutions envisaged

People

SQS Scientific Instrument

- Michael Meyer
- Thomas Baumann
- Alberto De Fanis
- Patrik Grychtol
- Markus Ilchen
- Tommaso Mazza
- Yevheniy Ovcharenko
- Haiou Zhang
- Paweł Ziolkowski

X-Ray Optics Group @XFEL

- Harald Sinn
 - Daniele La Civita
 - Maurizio Vannoni
 - Liubov Samoloyova
- FMB Oxford** 
- Richard Green, Kevin Mayo, Scott Mowat, Lucy Stock, Adam Young

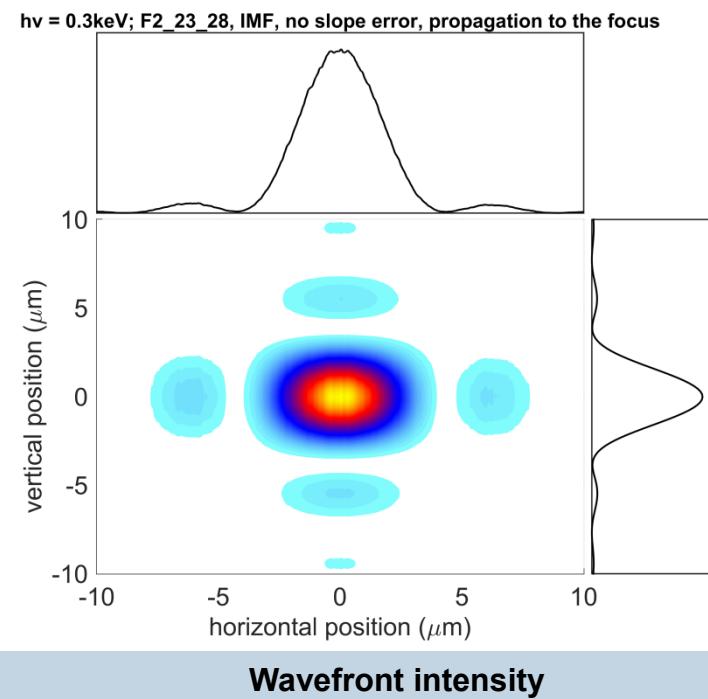
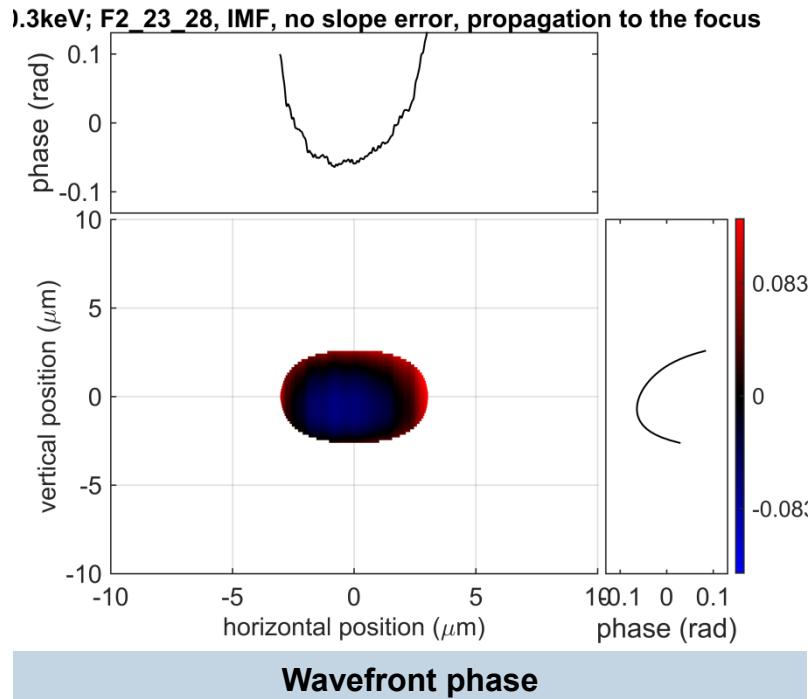
Elettra

- Luca Rebuffi

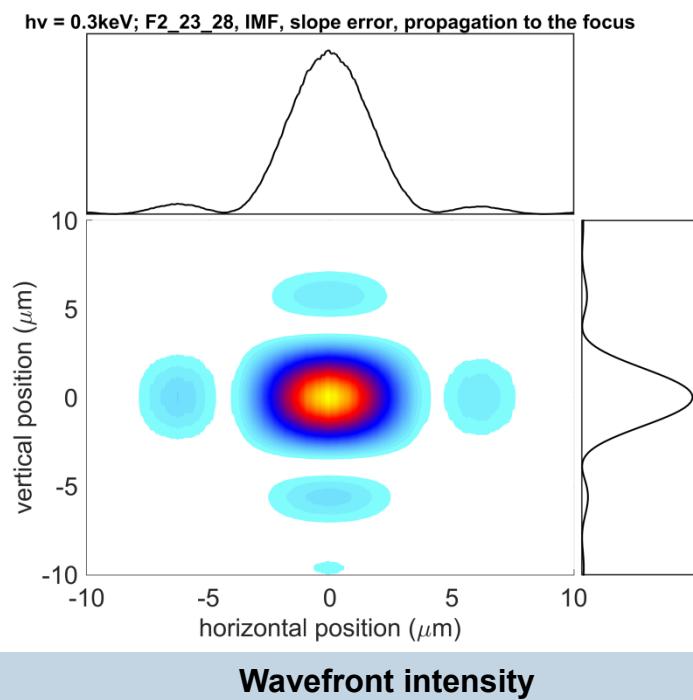
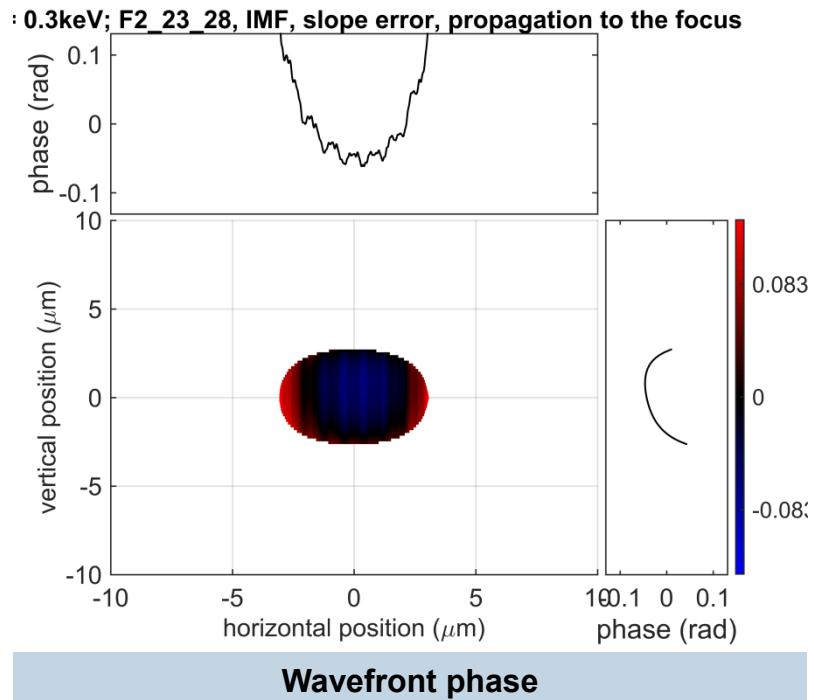
Additional information / topic

- Detuning dependence
- Rayleigh lengths
- Wavefront simulation for all scenarios
- Radiation dose
- Handling the gravitational sag
- Effect of thermal bump under extreme conditions
- Move also image for interim solution – how does it work

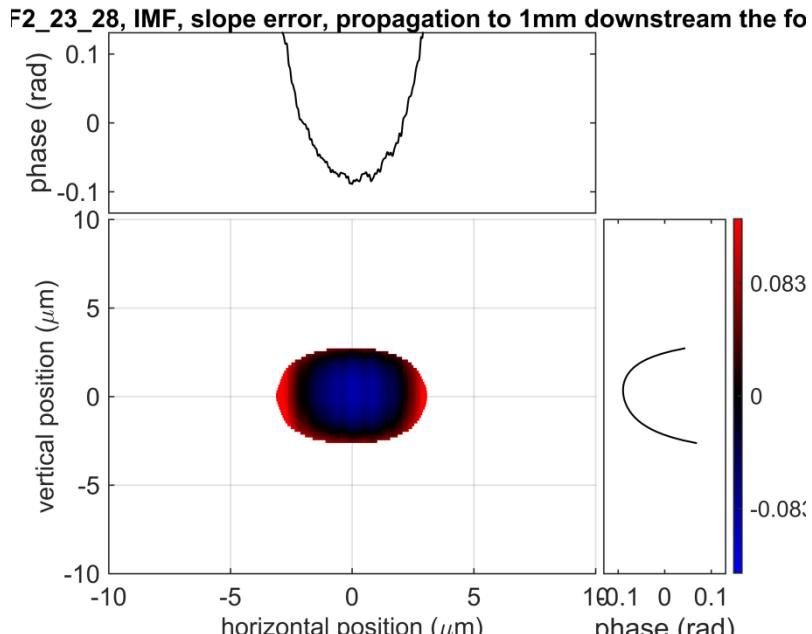
Wavefront in F2 – H IMF, CA=400; V DF, CA=600, w/o sl. err $h\nu = 300\text{eV}$, in focus



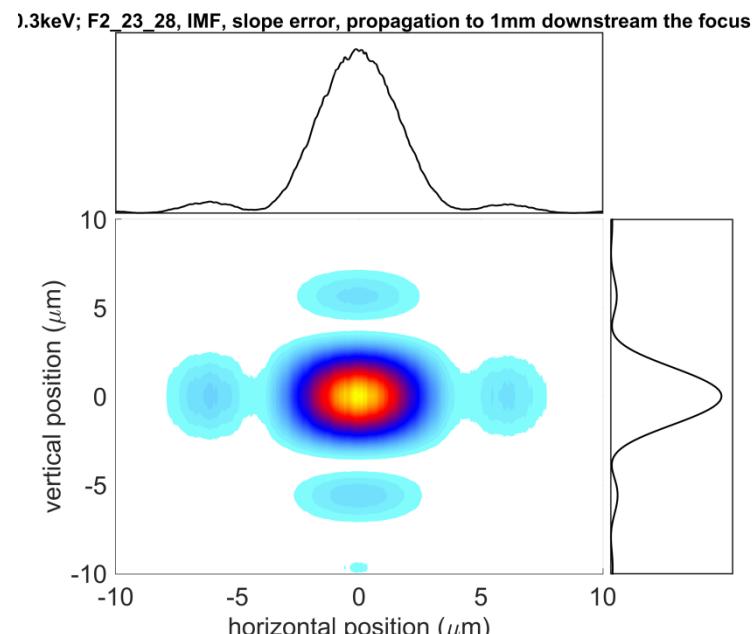
Wavefront in F2 – H IMF, CA=400; V DF, CA=600, with sl. err $h\nu = 300\text{eV}$, in focus



Wavefront in F2 – H IMF, CA=400; V DF, CA=600, with sl. err $h\nu = 300\text{eV}$, 1mm out of focus

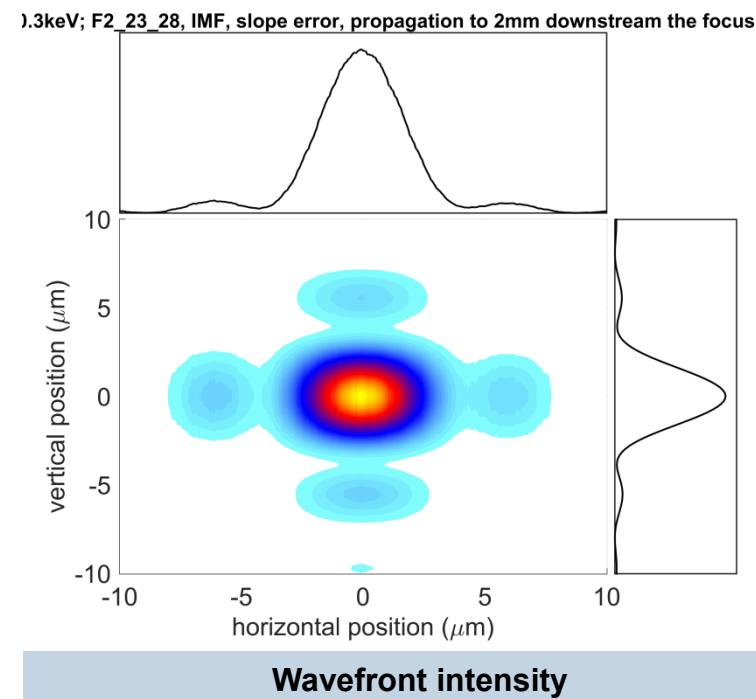
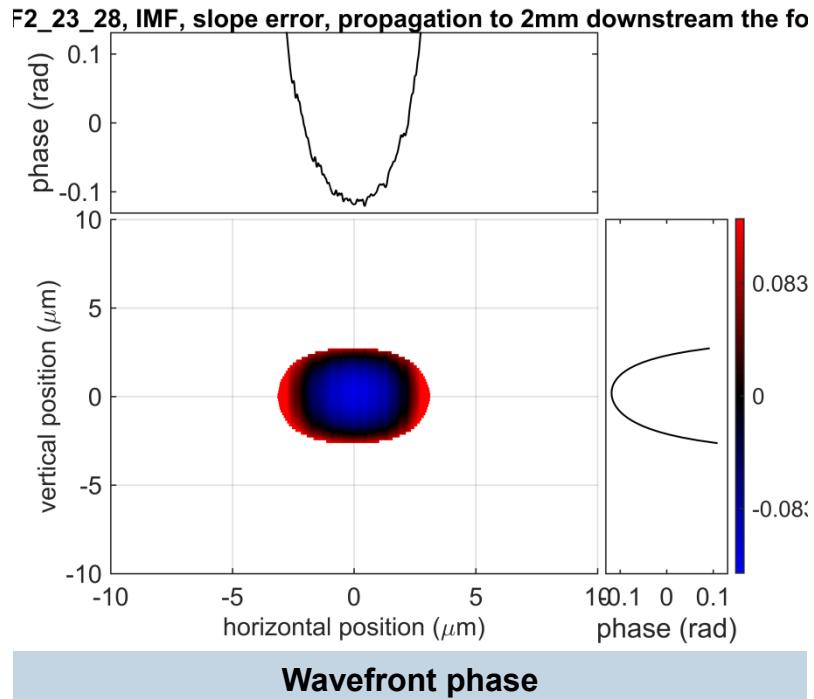


Wavefront phase

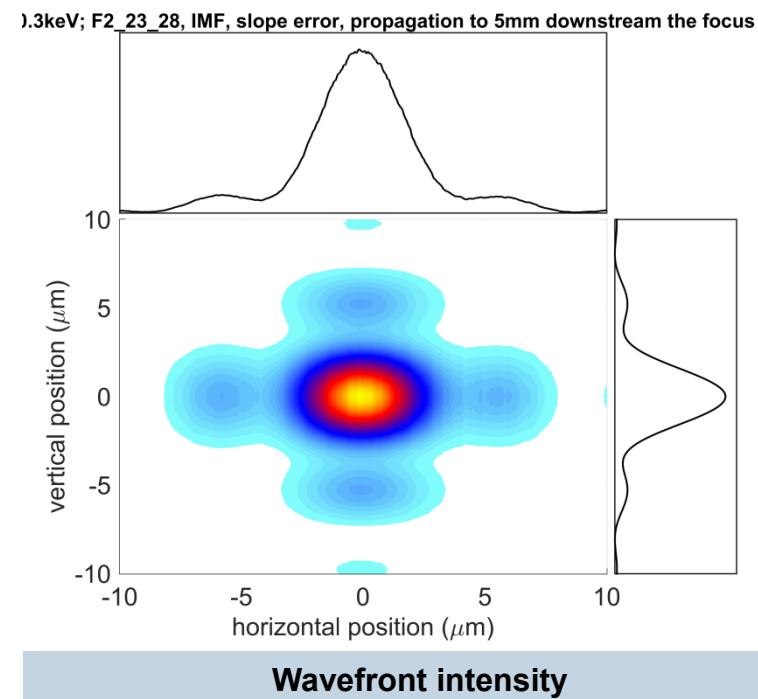
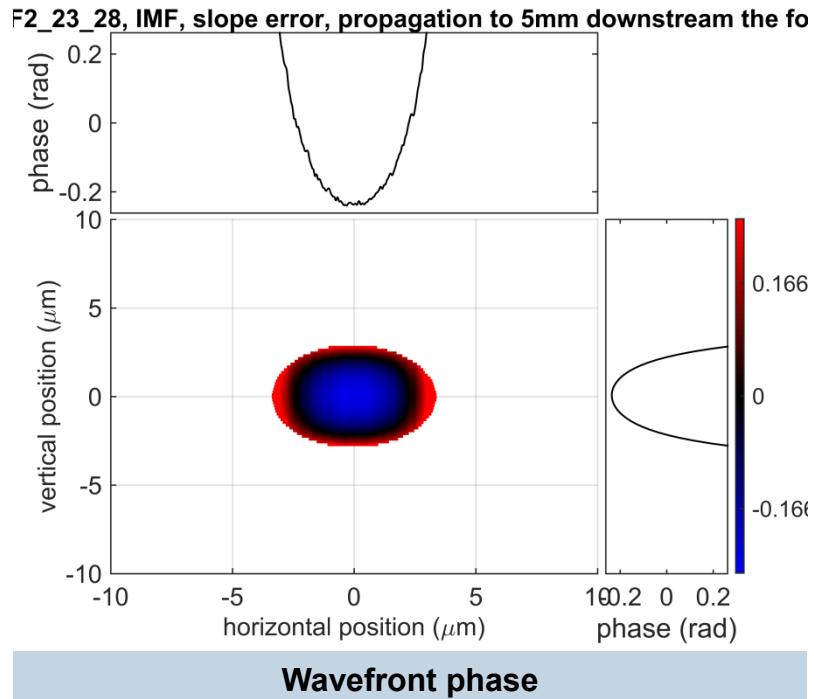


Wavefront intensity

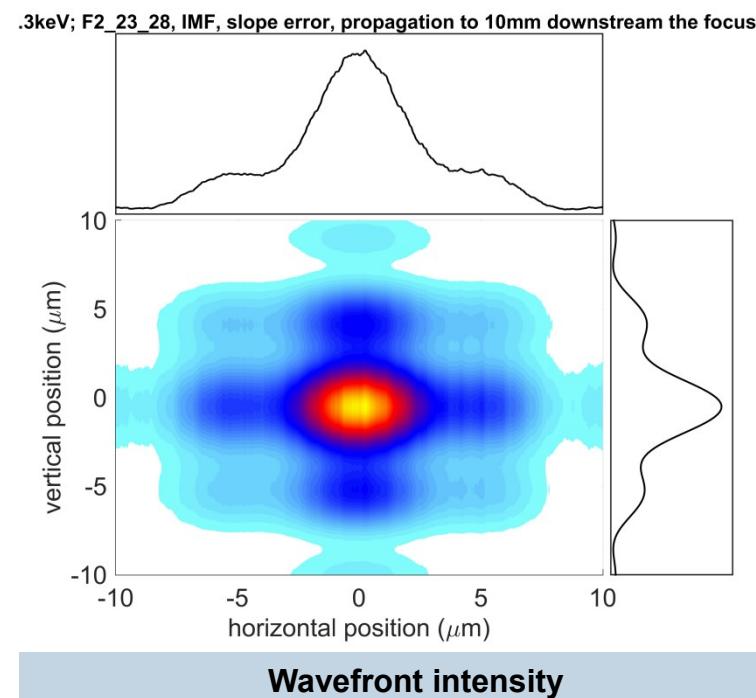
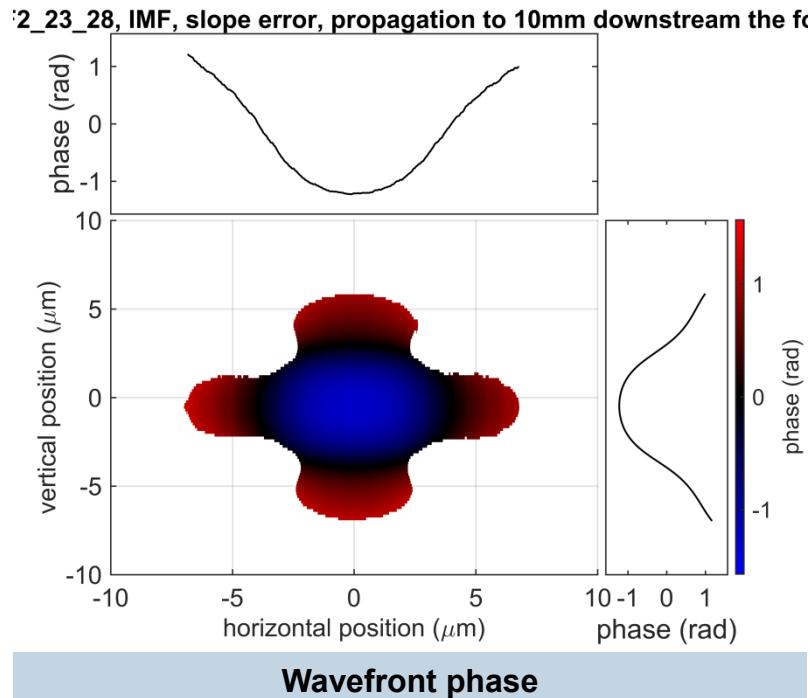
Wavefront in F2 – H IMF, CA=400; V DF, CA=600, with sl. err $h\nu = 300\text{eV}$, 2mm out of focus



Wavefront in F2 – H IMF, CA=400; V DF, CA=600, with sl. err $h\nu = 300\text{eV}$, 5mm out of focus



Wavefront in F2 – H IMF, CA=400; V DF, CA=600, with sl. err $h\nu = 300\text{eV}$, 10mm out of focus



Ray tracing: Focusing performances in F1 including thermal load

