Wave-optical simulations of focusing x-ray multilayer mirrors

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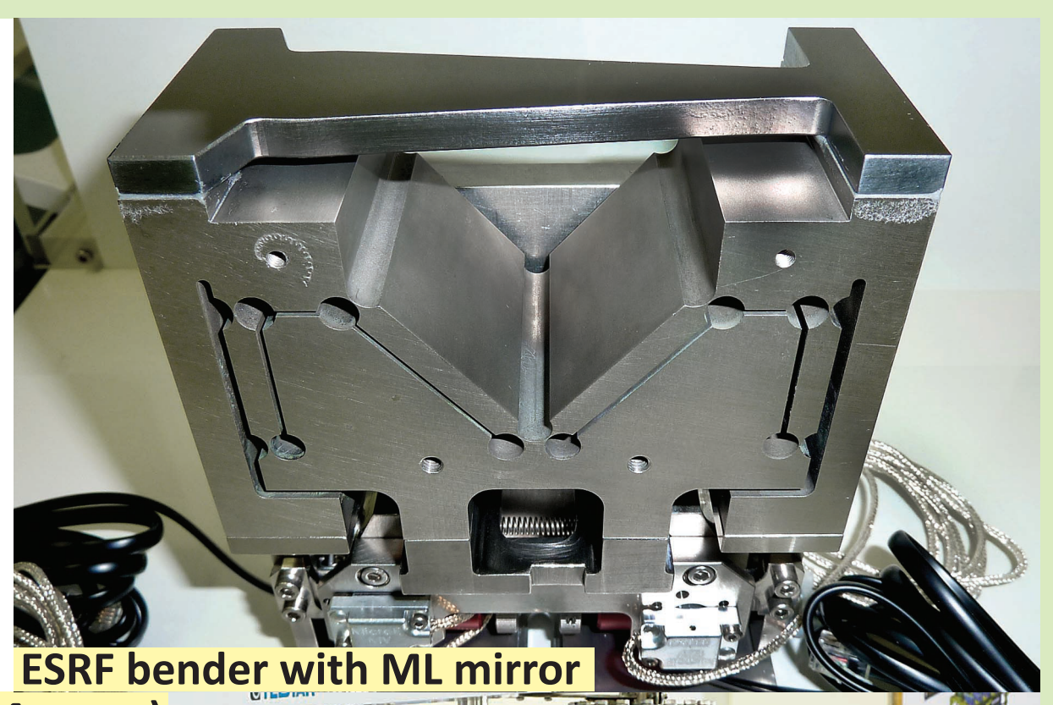
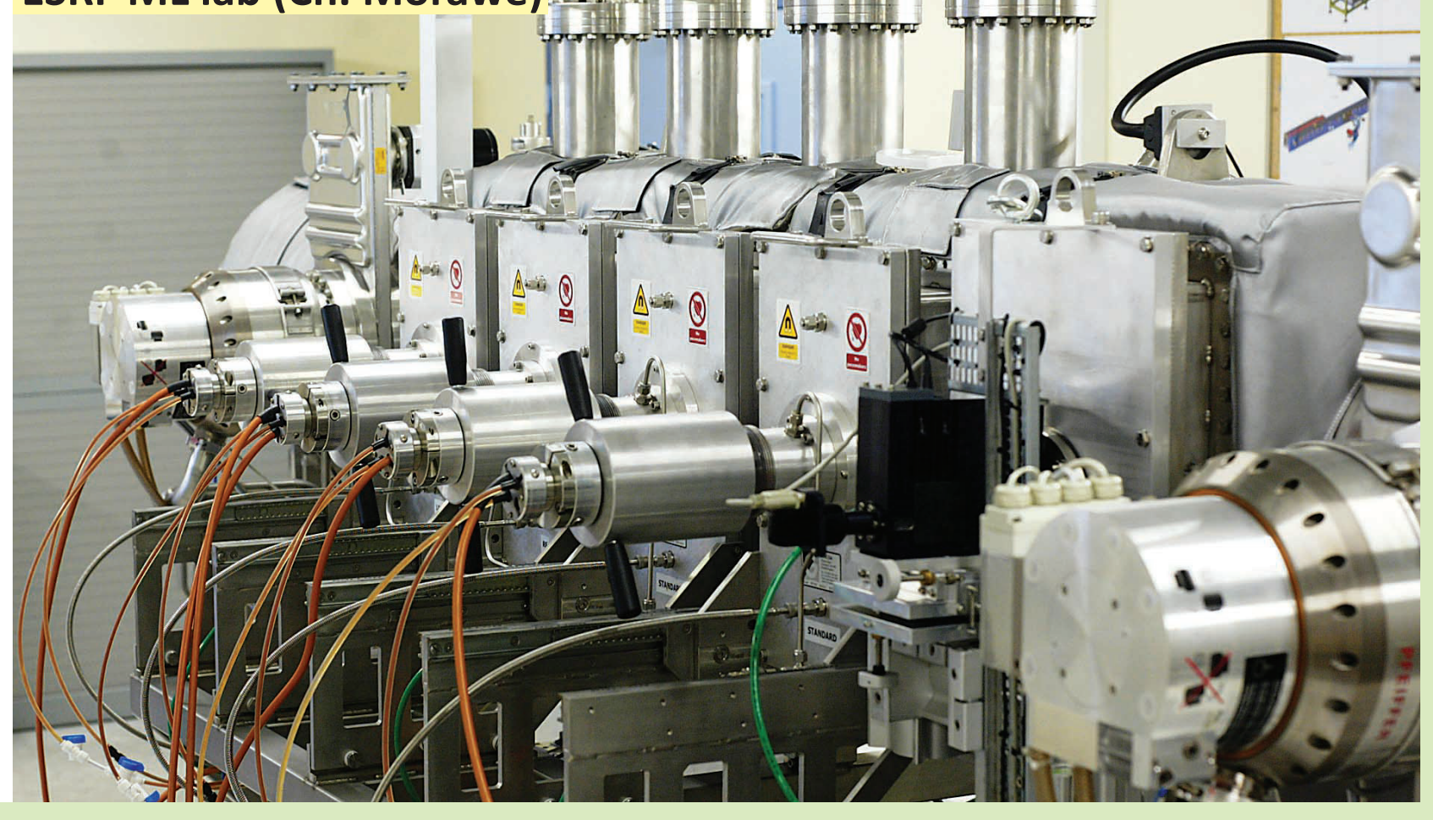
Focusing down to the nano metre

- X-rays: wavelengths below the nano metre scale
- but usually the numerical aperture is very small
- focus sizes: typically a few hundred nanometres,

world records:
20 to 50 nm in 2D (different techniques)
7 nm in 1D [1]



ESRF bender with ML mirror



ESRF ML lab (Ch. Morawe)

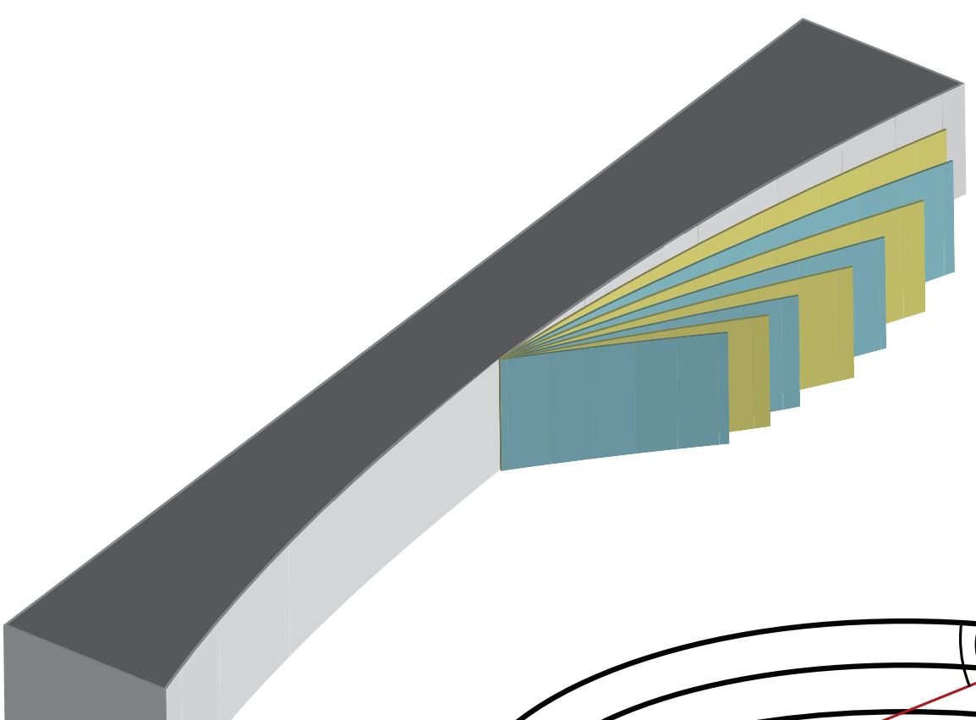
What we need:

- "large" numerical aperture, e.g. ≥ 0.01
- high reflectivity

(One possible) solution:
multilayer mirrors, as built at the ESRF (ML lab, Christian Morawe) [2]

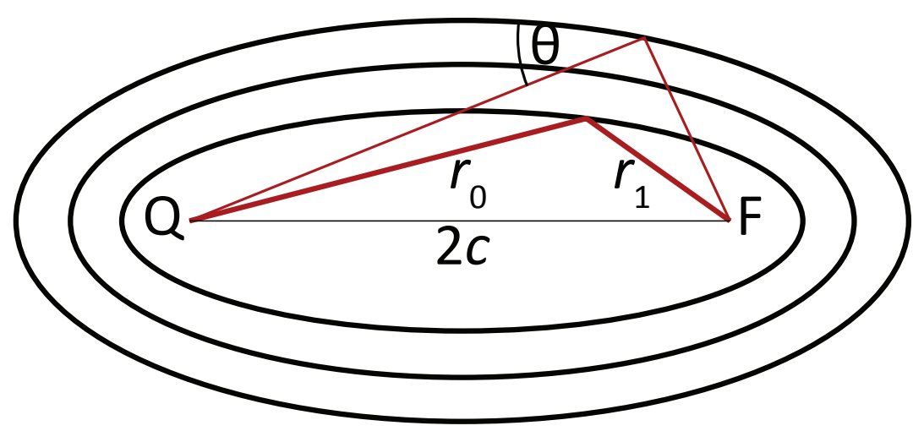
Focusing multilayer mirrors

- alternating layers of high optical contrast
- typical layer thicknesses: 1 to 4 nanometres
- typical layers: $(\mathrm{W} / \mathrm{B_4C})_{25\ldots100}$
- typical angles of incidence: 5 to 15 milliradians



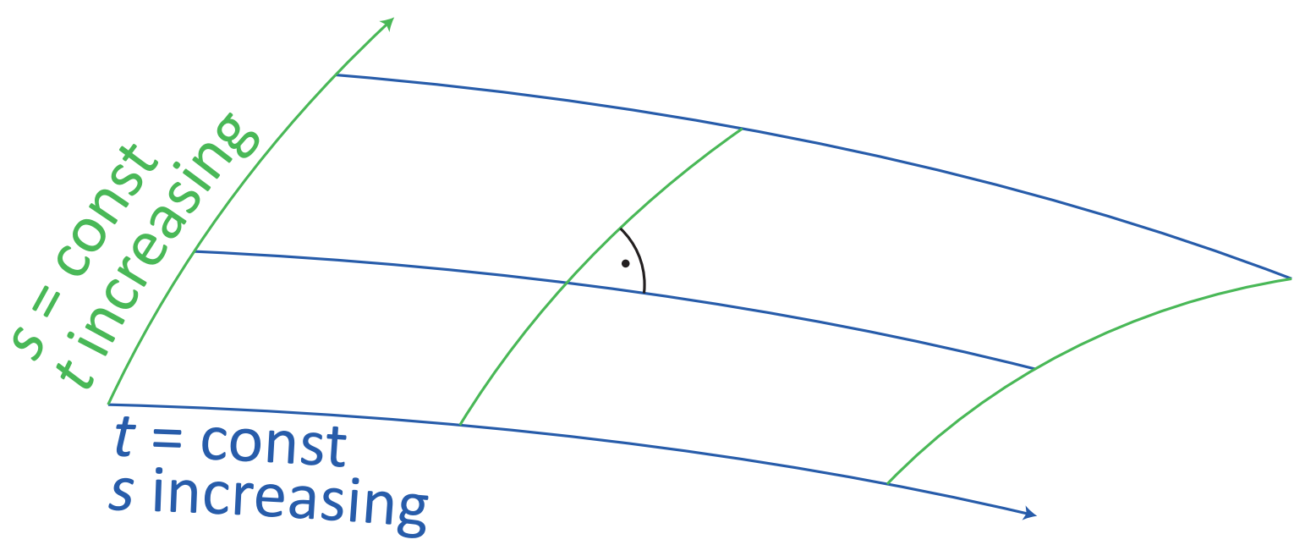
Elliptical shapes

- total reflection mirrors: single ellipse
- multilayers: (nearly) confocal ellipses
- convenient analytical description: elliptical coordinates



Elliptical Takagi-Taupin

- two wave-fields (incoming and reflected)
- Fourier series of susceptibility
- cylindrical waves, slowly varying envelopes, elliptical coordinates



Modified Bragg equation

- refraction occurs inside "averaged" medium
- phases of reflected waves do not match
- modified layer thickness Λ: $\Lambda^{\mathrm{mB}} = \lambda/2\,\sqrt{n^2 - \cos^2\theta}$ [2]

Takagi-Taupin theory, fundamentals:

- incoming wave: ψ_0
- reflected wave: ψ_1
- Fourier series of susceptibility: χ_0, χ_{-1}, χ_{+1}

$$(\alpha^2\partial_s + \beta^2\partial_t)\psi_0 = i\left(u_0\psi_0 + u_1\psi_1\right) - \gamma^+\psi_0,$$
$$(\alpha^2\partial_s - \beta^2\partial_t)\psi_1 = i\left(u_0\psi_1 + u_{\bar{1}}\psi_0\right) + \gamma^-\psi_1$$

In curved geometry:

- finite differences on regular grid
- spatially dependant coefficients α, β describe geometry
- γ-terms due to cylindrical waves
- local angle of incidence $\vartheta(s,t)$

$$\alpha^2 = \frac{c^2 - s^2}{t^2 - s^2}, \quad \beta^2 = \frac{t^2 - c^2}{t^2 - s^2}$$
$$2\gamma^\pm = \pm\frac{1}{t \pm s}, \quad u_h = k\chi_h/2$$

[3]

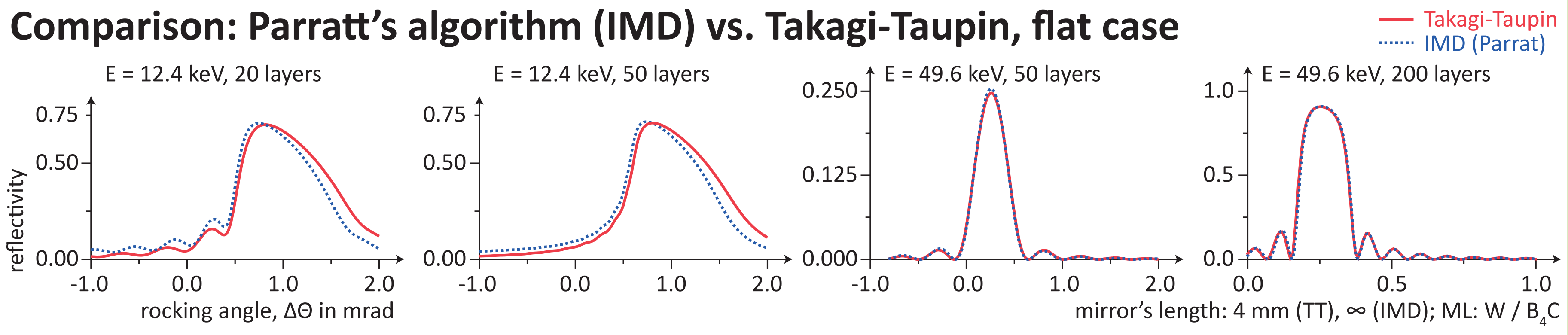
Modified Bragg equation:

- local correction
- increased layer thickness
- "anti-phase shift" of reflected wave
- motivated by geometrical considerations, *now: wave-optical confidence*

$$(\alpha^2\partial_s + \beta^2\partial_t)\,\psi_0 = i\left(+u_0\psi_0 + u_{\bar{1}}\psi_1\right) - \gamma^+\psi_0,$$
$$(\alpha'^2\partial_s - \beta'^2\partial_t)\,\psi_1 = i\left(-u_0\psi_1 + u_1\psi_0\right) + \gamma'^-\psi_1,$$
$$\alpha'^2 = \alpha^2, \qquad \beta'^2 = \beta^2(1 - 2\delta/\sin^2\theta).$$

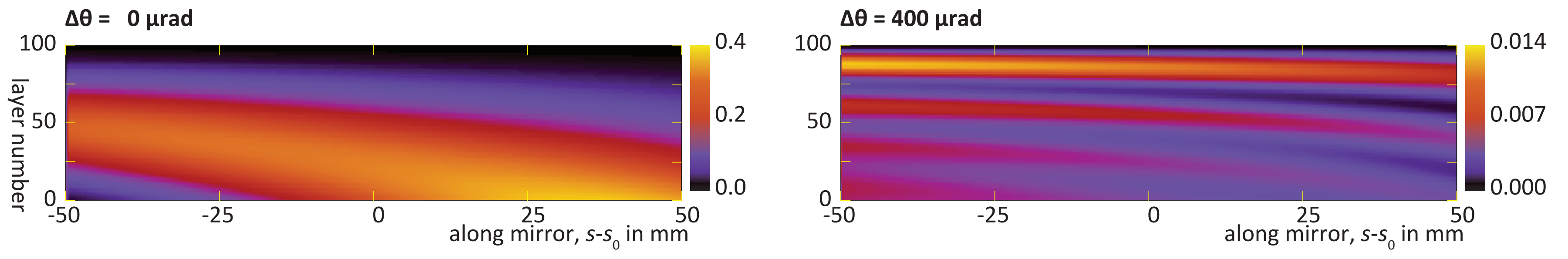
[4]

Comparison: Parratt's algorithm (IMD) vs. Takagi-Taupin, flat case



mirror's length: 4 mm (TT), ∞ (IMD); ML: $\mathrm{W / B_4C}$

Elliptical TT: reflected intensity



only part of the curved mirror reaches maximum reflection

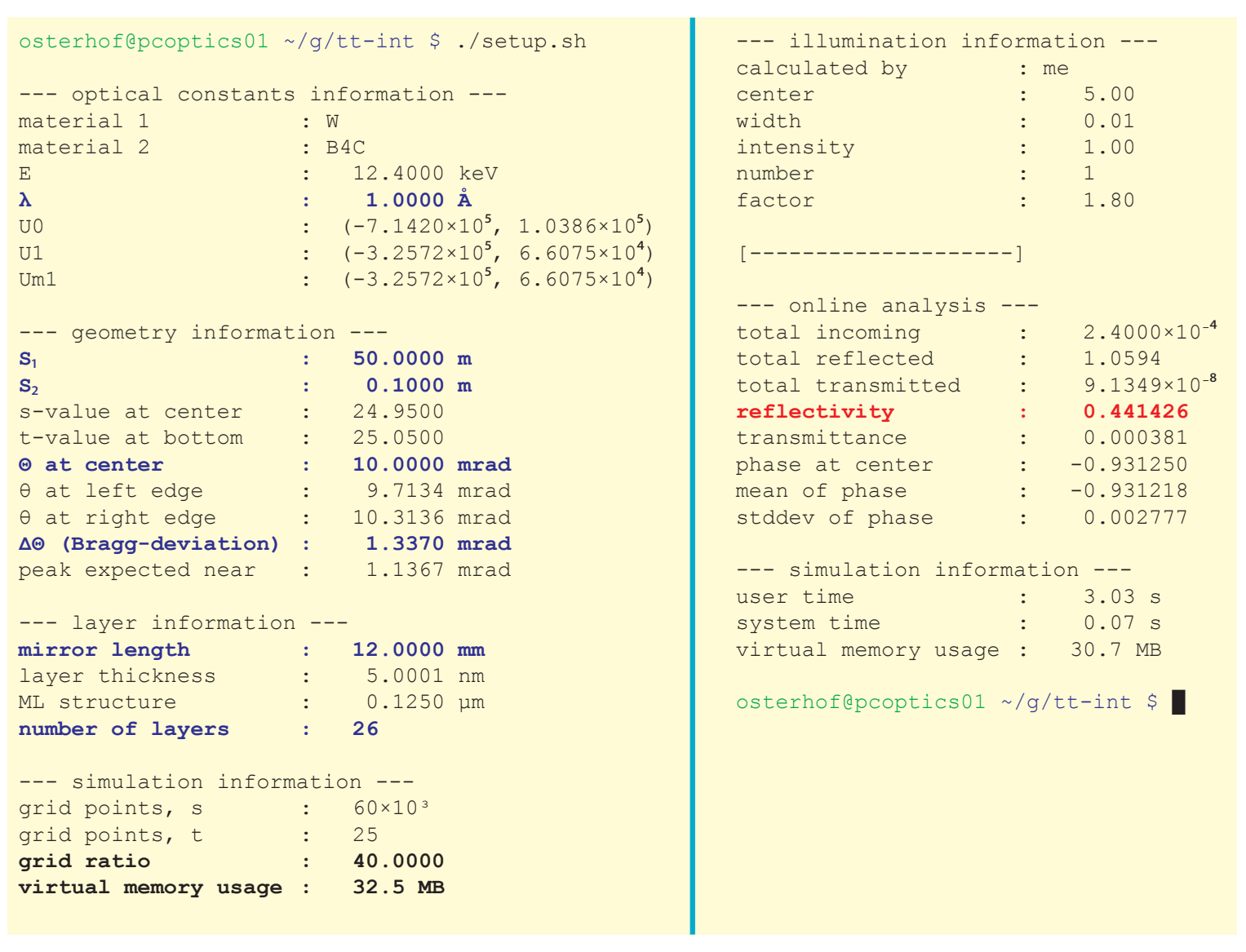
completely mis-tuned mirror

photon energy: 12.4 keV
source distance: 50.0 m

focal length: 100 mm
Bragg angle: 10.0 mrad

ML structure: $(\mathrm{W / B_4C})_{100}$

X-ray MultiLayer Simulations



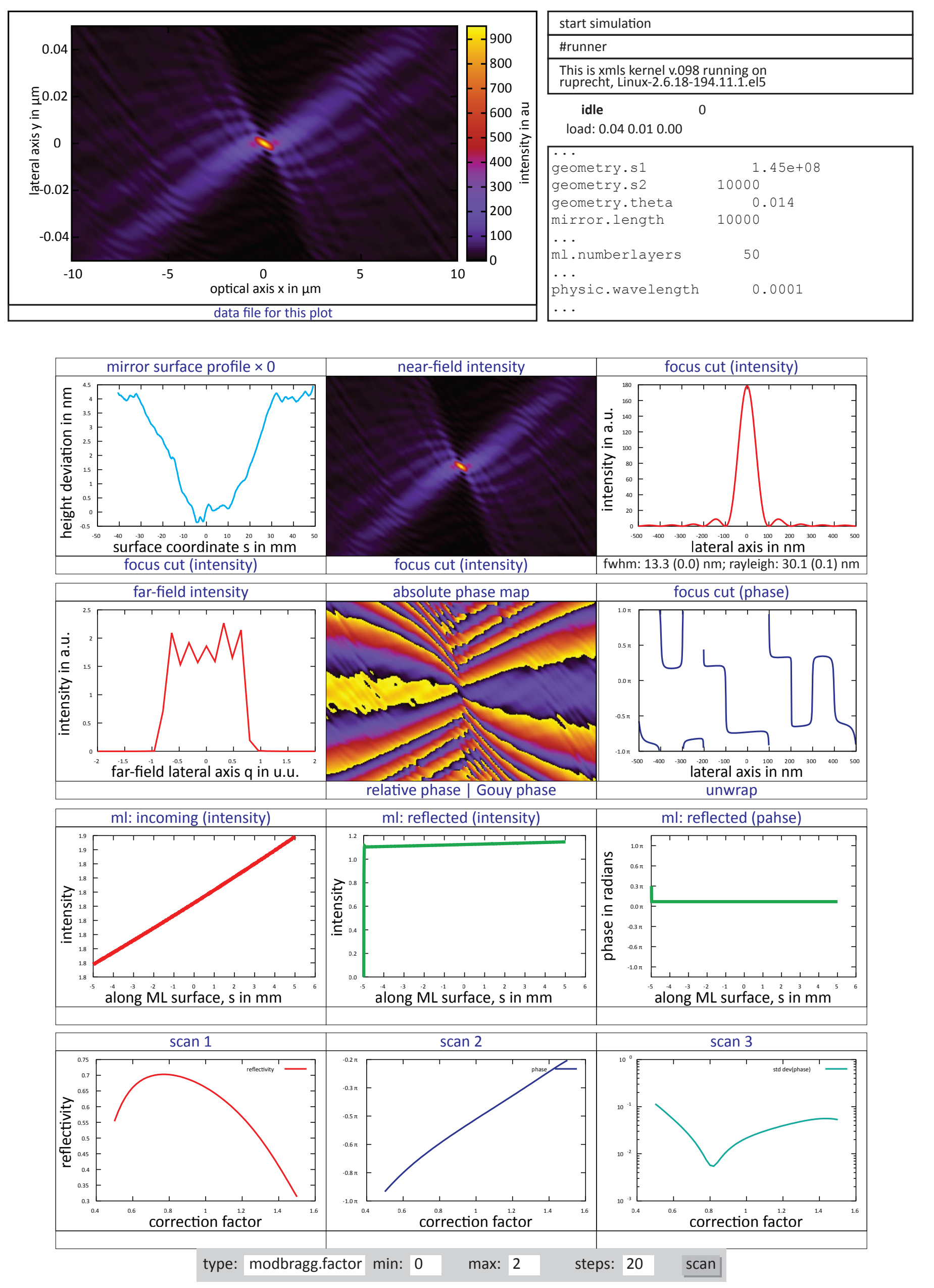
```
osterhof@pcoptics01 ~/g/tt-int $ ./setup.sh

--- optical constants information ---
material 1            : W
material 2            : B4C
E                     :   12.4000 keV
λ                     :    1.0000 Å
U0                    :  (-7.1420×10⁵, 1.0386×10⁵)
U1                    :  (-3.2572×10⁵, 6.6075×10⁴)
Um1                   :  (-3.2572×10⁵, 6.6075×10⁴)

--- geometry information ---
S₁                    :   50.0000 m
S₂                    :    0.1000 m
s-value at center     :   24.9500
t-value at bottom     :   25.0500
Θ at center           :   10.0000 mrad
θ at left edge        :    9.7134 mrad
θ at right edge       :   10.3136 mrad
ΔΘ (Bragg-deviation)  :    1.3370 mrad
peak expected near    :    1.1367 mrad

--- layer information ---
mirror length         :   12.0000 mm
layer thickness       :    5.0001 nm
ML structure          :    0.1250 µm
number of layers      :   26

--- simulation information ---
grid points, s        :   60×10³
grid points, t        :   25
grid ratio            :   40.0000
virtual memory usage  :   32.5 MB
```

```
--- illumination information ---
calculated by          : me
center                 :    5.00
width                  :    0.01
intensity              :    1.00
number                 :    1
factor                 :    1.80

[--------------------]

--- online analysis ---
total incoming         :    2.4000×10⁻⁴
total reflected        :    1.0594
total transmitted      :    9.1349×10⁻⁸
reflectivity           :    0.441426
transmittance          :    0.000381
phase at center        :   -0.931250
mean of phase          :   -0.931218
stddev of phase        :    0.002777

--- simulation information ---
user time              :    3.03 s
system time            :    0.07 s
virtual memory usage   :   30.7 MB

osterhof@pcoptics01 ~/g/tt-int $ █
```

Using XMLS

- flexible command line interface allowing for loops and hooks
- GUI implemented by webserver: control simulation from your browser, fully remote-controlled and independent of control PC's capabilities
- control simulations and access data even from third party software (using HTTP)

webGUI: control online, calculate anywhere



start simulation

#runner

This is xmls kernel v.098 running on ruprecht, Linux-2.6.18-194.11.1.el5

idle 0
load: 0.04 0.01 0.00

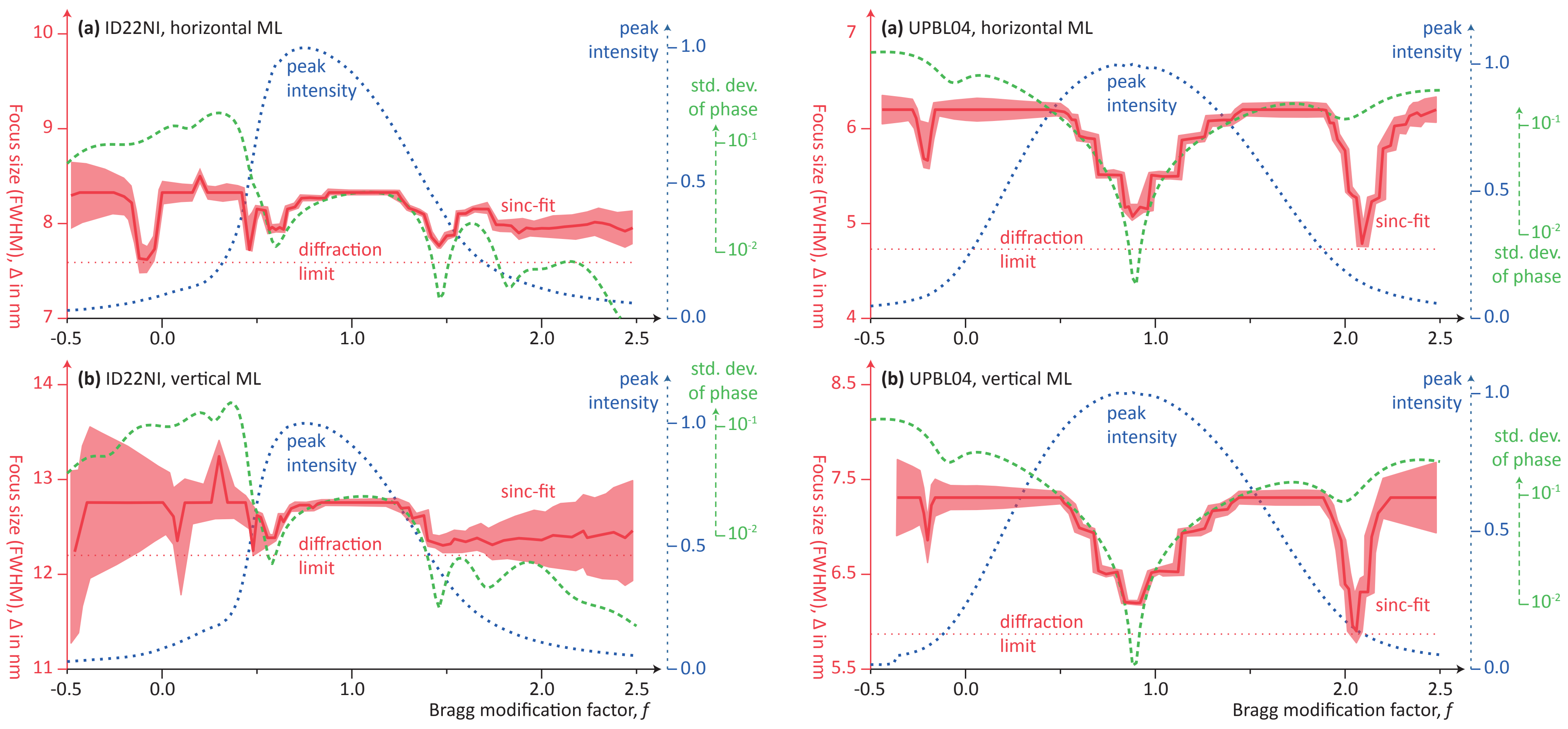
```
...
geometry.s1             1.45e+08
geometry.s2          10000
geometry.theta          0.014
mirror.length        10000
...
ml.numberlayers        50
...
physic.wavelength       0.0001
...
```

fwhm: 13.3 (0.0) nm; rayleigh: 30.1 (0.1) nm

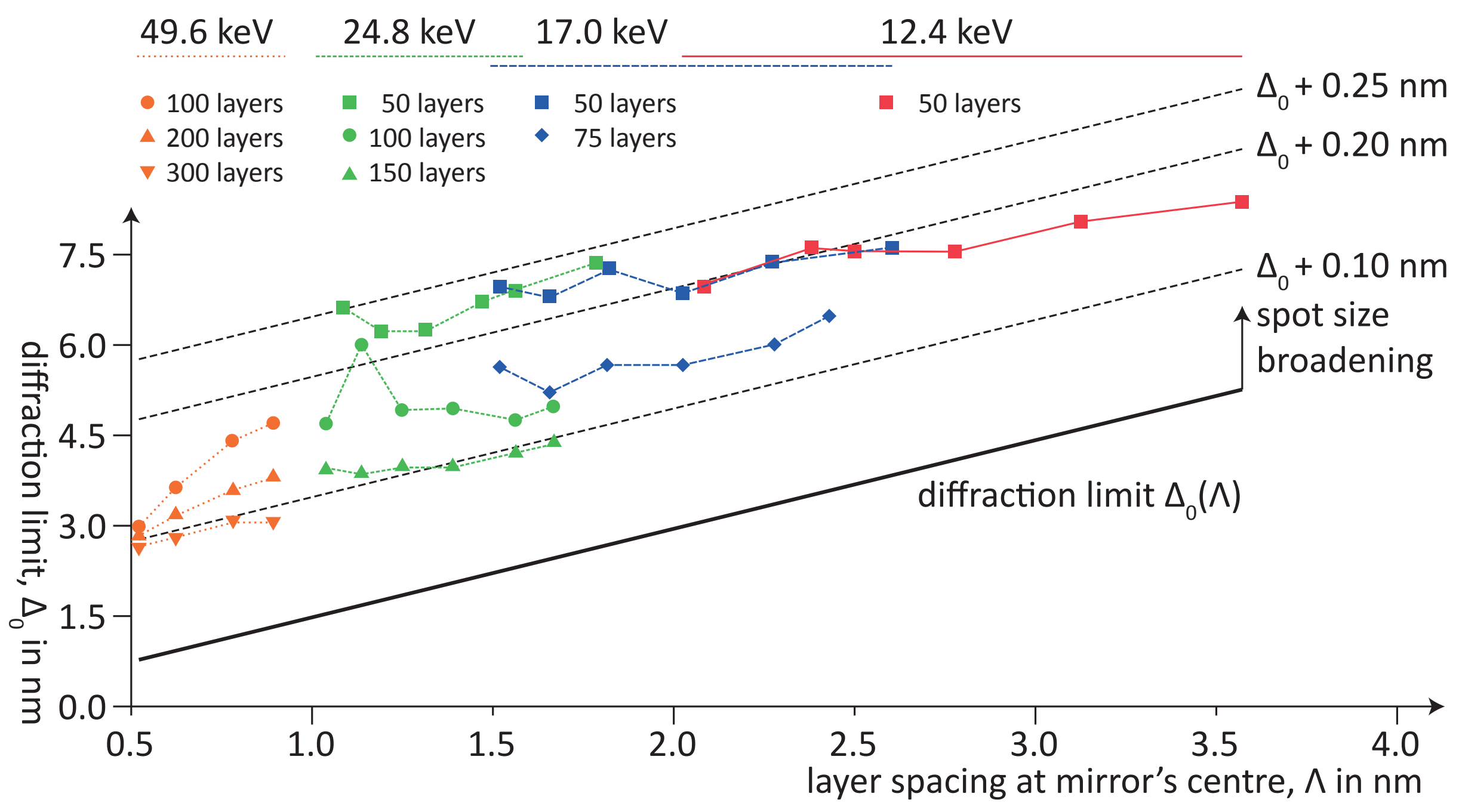
type: modbragg.factor min: 0 max: 2 steps: 20

(reproduced screenshot from Mozilla Firefox)

New ESRF multilayer mirrors



No fundamental limits (within this model)



Propagating the reflected field to the focal region allows for estimating the focus properties of next-generation ML focusing mirrors.

top row:

Numerical optimisation of the layer shapes promises focus sizes below the 10 nm scale (for a point-source) for the NINA branch of ESRF's new UPBL04 beamline.

left:

A model system going beyond what is possible to fabricate shows no fundamental limits of the proposed analytical scheme below focus sizes smaller than 1 nm.

Summary

- Wave-optical theory / numerical code describing focusing multilayer mirrors
- Optimisation of next-generation optics
- Model allows for sub-nm focus sizes

Outlook

- real structure effects:
  surface roughness / figure errors / errors inside the structure
- partially coherent sources
- polychromaticity / short bunches

Related publications

References

[1] H. Mimura, et al, "Breaking the 10 nm barrier in hard-X-ray focusing", Nature Physics 6 (2010).
[2] Ch. Morawe, M. Osterhoff, "Curved graded multilayers for X-ray nano-focusing optics", NIM A 616 (2010).
[3] M. Osterhoff et al, submitted / PhD thesis (2012).
[4] M. Osterhoff et al, in preparation / PhD thesis (2012).