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concept
for a
reflectometer
using
focusing guides



Selene

TUM & FRM II seminar
12. 03. 2012, München, Germany

outline

reflectometry

- principle
- examples

slit optics vs. focusing optics

small samples

focusing with elliptic guides

- coma aberration
- operation modes

realisation

- add-on for Amor → experimental results
- 2D prototype for BOA
- concept for the ESS

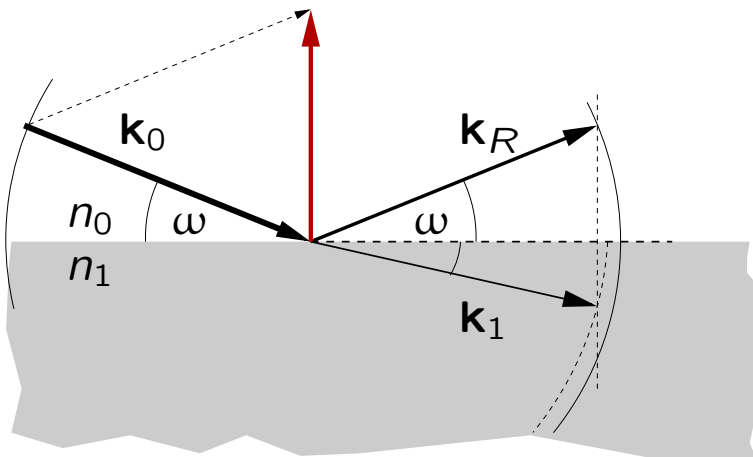
reflectometry

reflectometry



analogy to visible light:

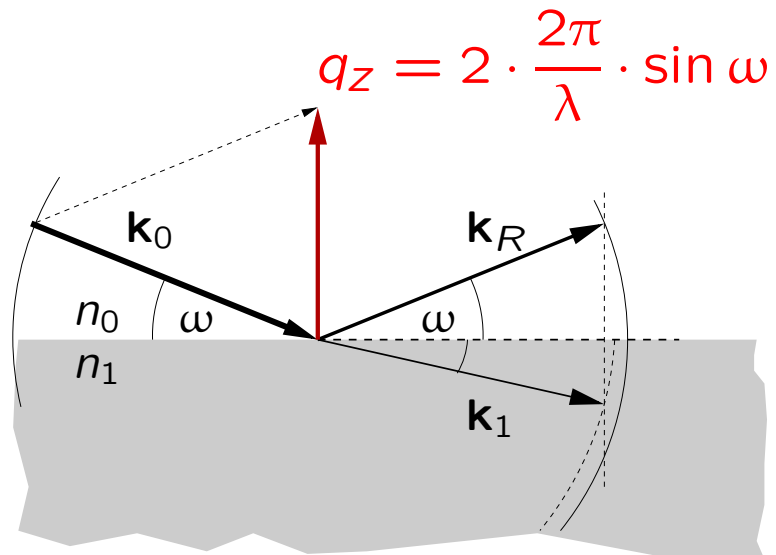
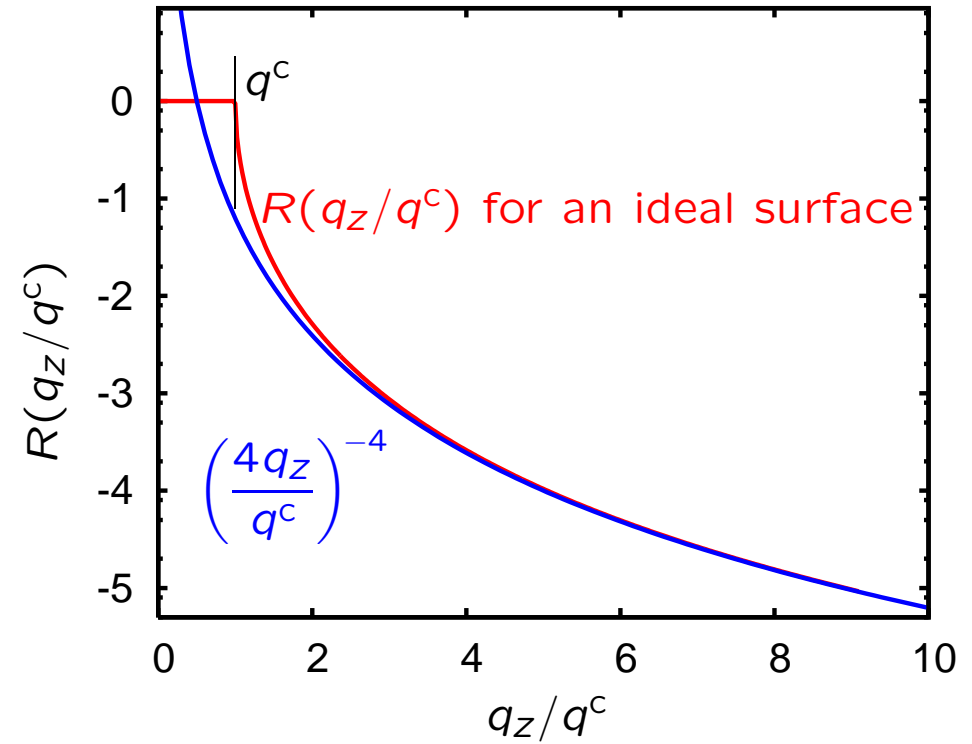
- *flat* surfaces partly reflect light
- some media also transmit light
- parallel interfaces \Rightarrow interference



reflectometry

Fresnel reflectivity

- reflectivity of a sharp flat surface
- total external reflection for $q_z < q^c$
- exponential decay of $R(q_z)$ for $q_z > q^c$



neutrons / x-rays:

$$\lambda \in \{1 \dots 20 \text{ \AA}\}$$

$$\omega^c < 1^\circ$$

reflectometry

reflected intensity of a multilayer

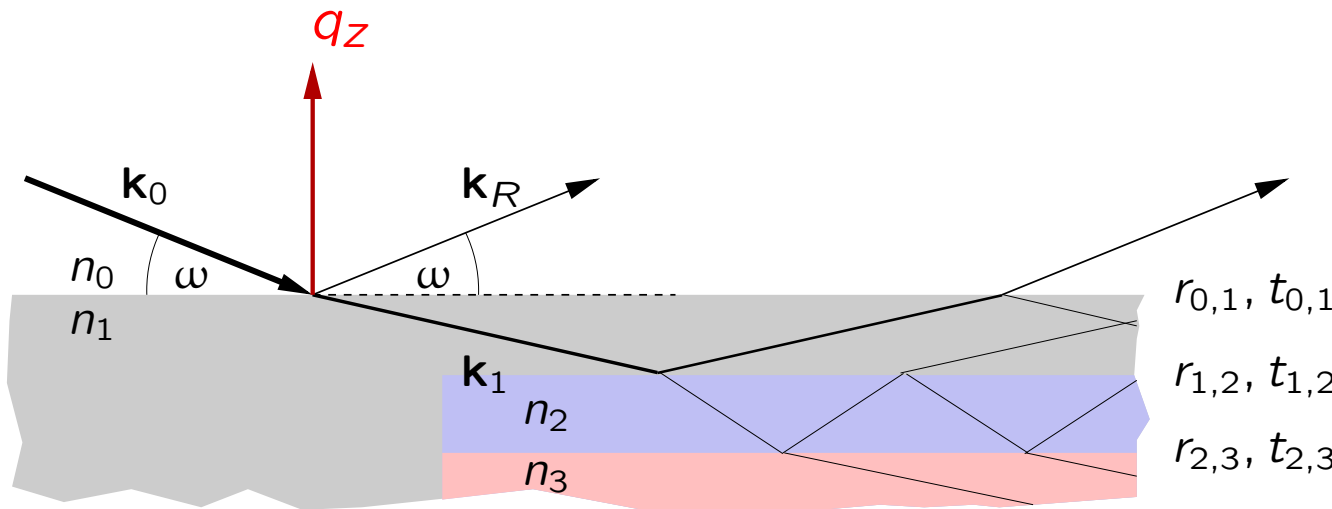
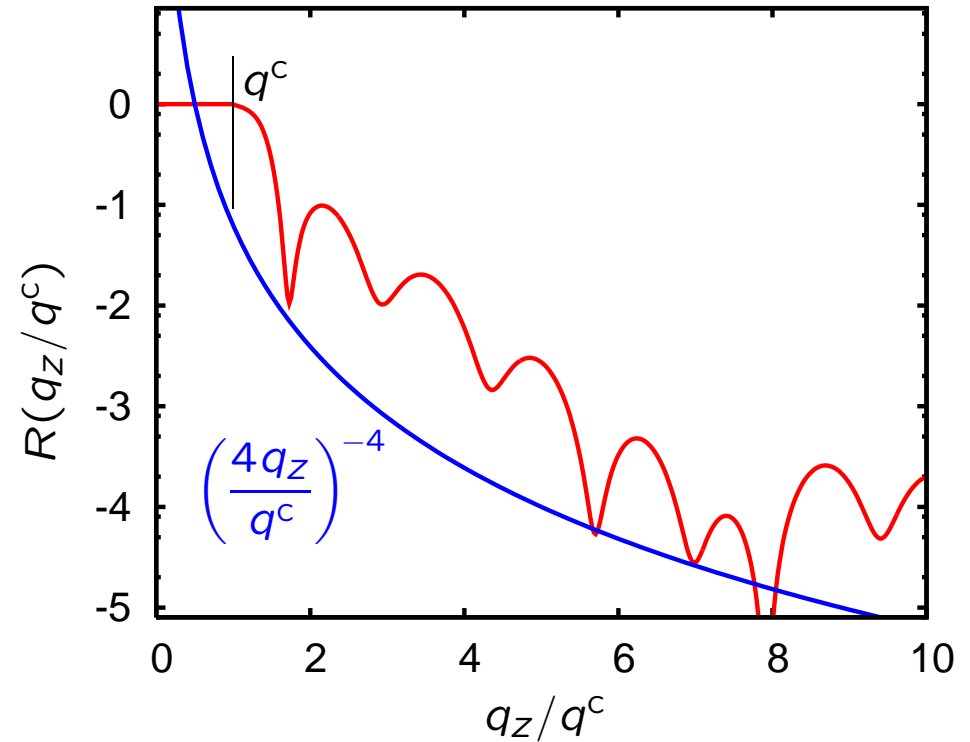
several parallel interfaces:

interference of all waves

⇒ complex reflectance

$$r = r(q_z, n_0, n_1, n_2, \dots, d_1, d_2, \dots)$$

$$R(q_z) = |r(q_z)|^2$$



- $r_{0,1}, t_{0,1}$
- d_1 thickness of layer 1
- $r_{1,2}, t_{1,2}$
- d_2
- $r_{2,3}, t_{2,3}$ reflectance of interface 2/3
- d_3

reflectometry

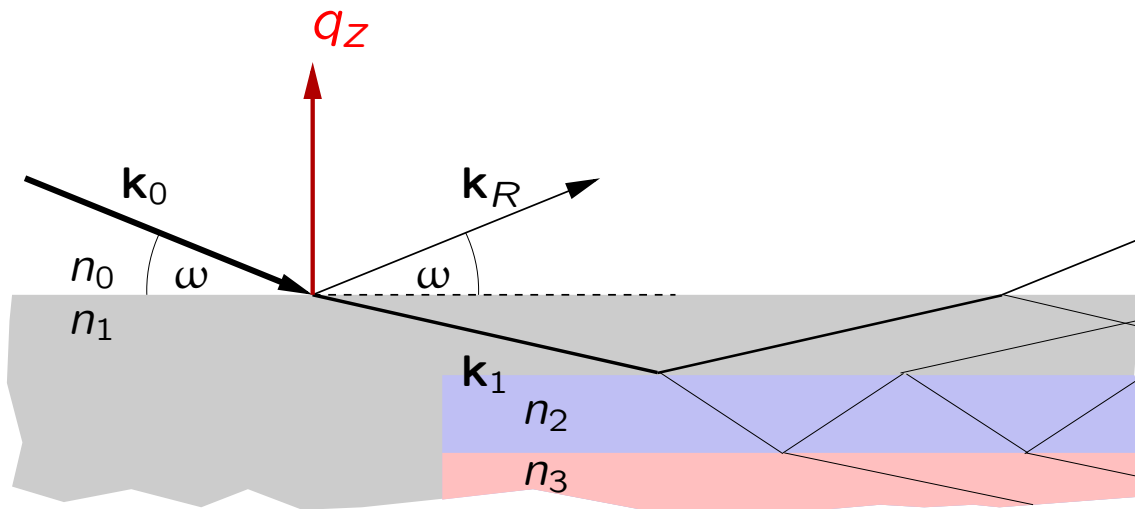
reflected intensity of a multilayer

$$R(q_z) = |r(q_z)|^2$$

⇒ all phase information is lost

⇒ one way road:

⇒ calculation of $R(q_z)$ using a model
and
comparison to measured curve(s)

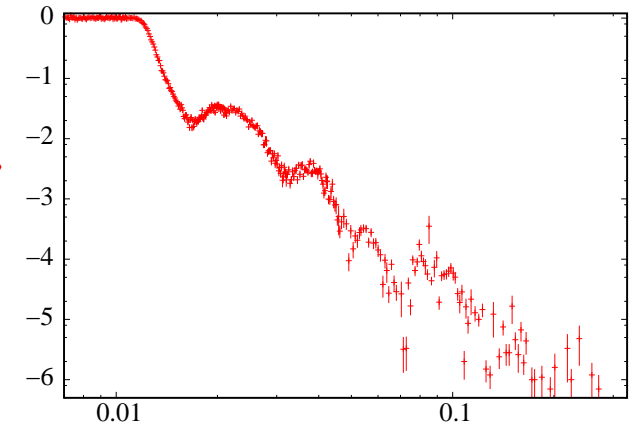
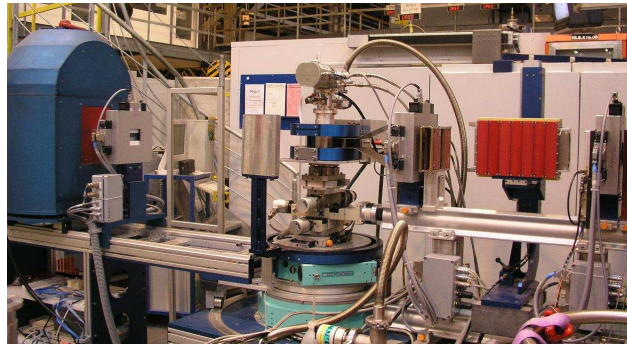
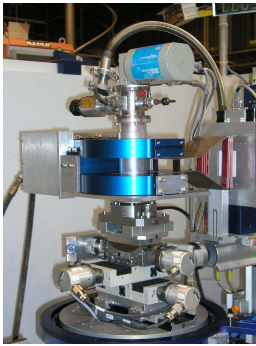


real effects

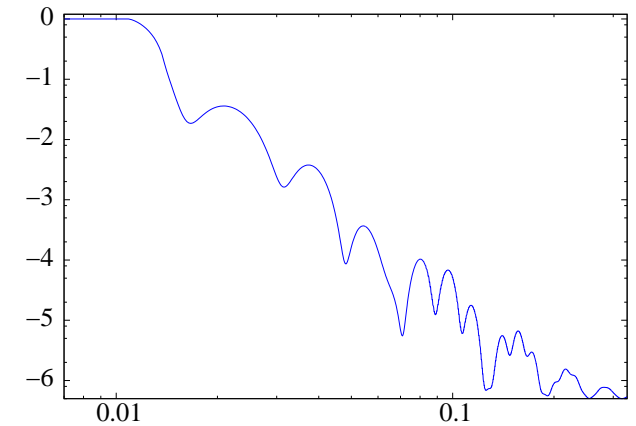
to be taken into account:

- illumination of the sample
- resolution of the set-up
 $\Delta\omega$, $\Delta\lambda$
- non-sharp interfaces
- inhomogeneous layers

reflectometry



?



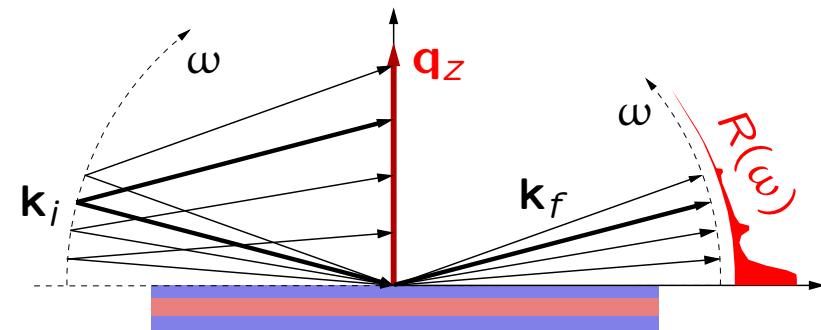
reflectometry

measurement schemes

$$R = R(q_z) = R(\lambda, \omega) \quad q_z = 4\pi \frac{\sin \omega}{\lambda}$$

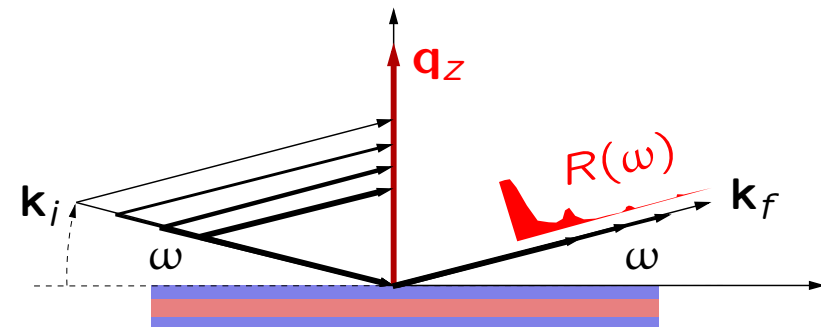
angle-dispersive set-up

variation of ω with fixed λ
 detection under 2ω



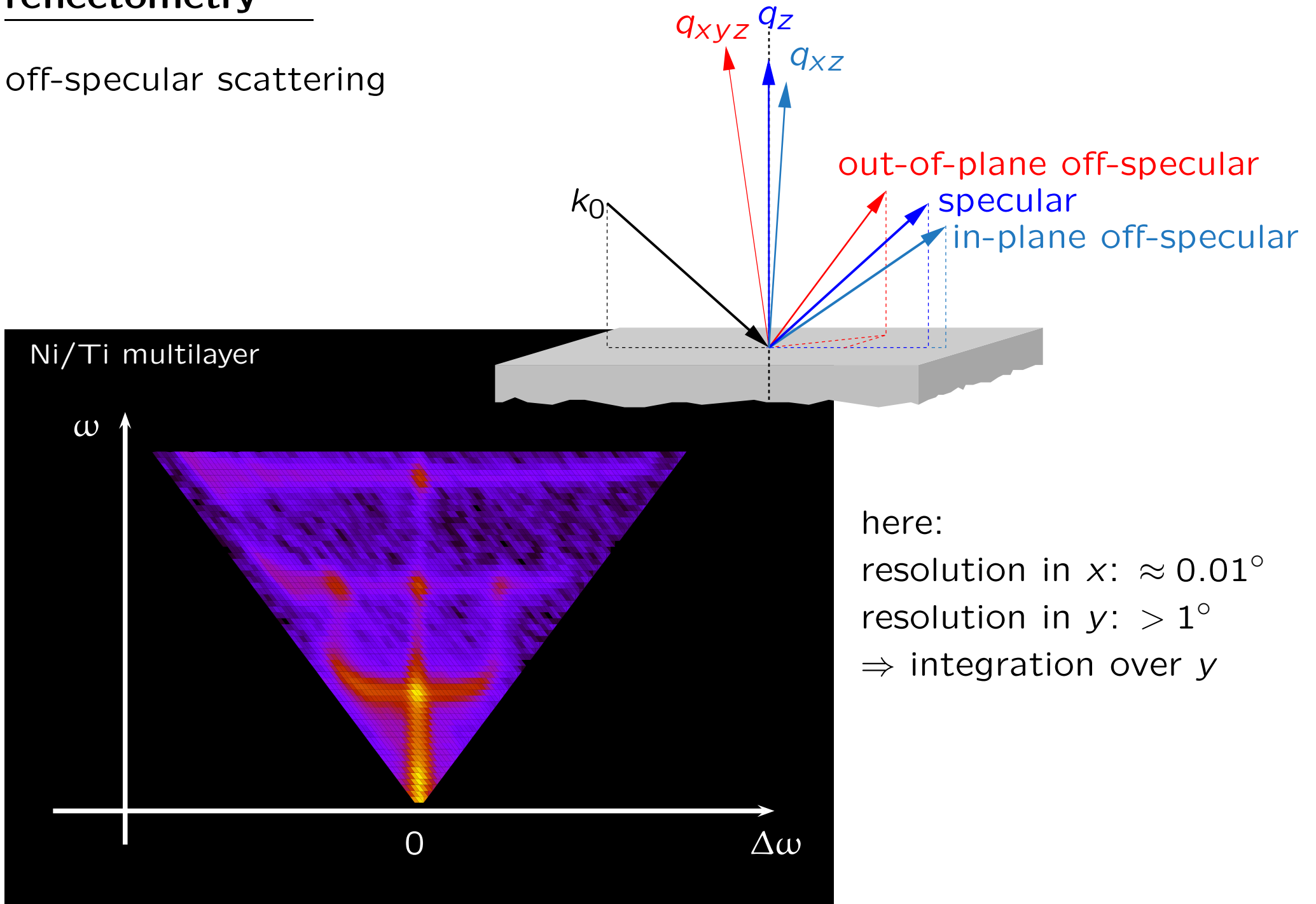
energy-dispersive set-up

variation of λ with fixed ω
 detection via time-of-flight



reflectometry

off-specular scattering



here:
resolution in x : $\approx 0.01^\circ$
resolution in y : $> 1^\circ$
 \Rightarrow integration over y

reflectometry

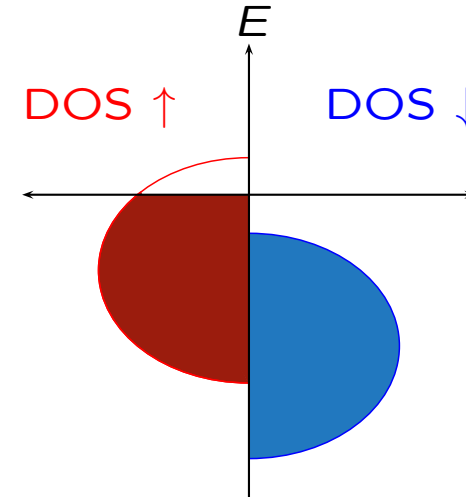
example: perovskite multilayer



LSMO is a half-metal

⇒ injection of spin-polarised current expected

→ but not found!



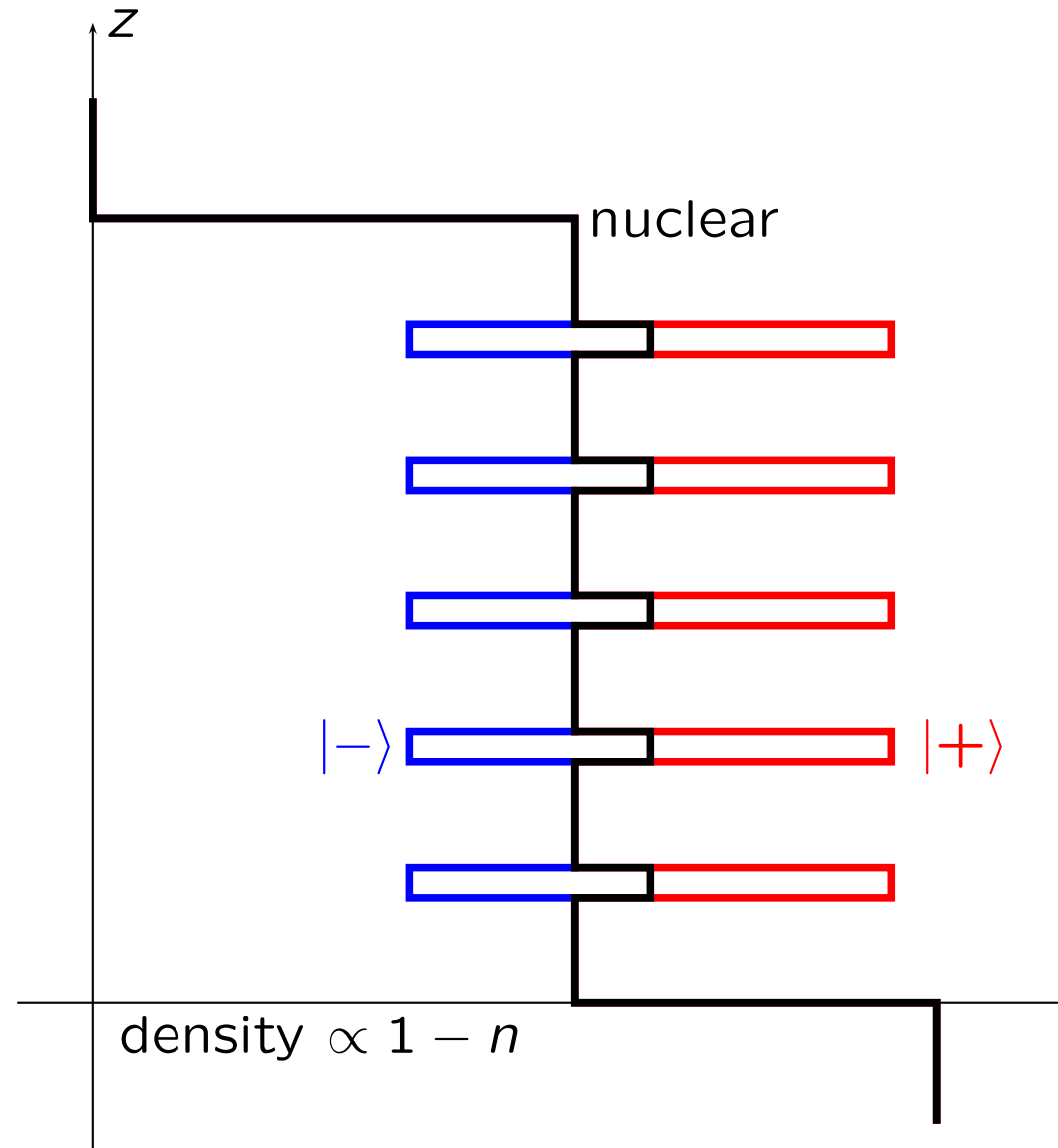
explanation: reduced / suppressed magnetism at interfaces

Is that true?

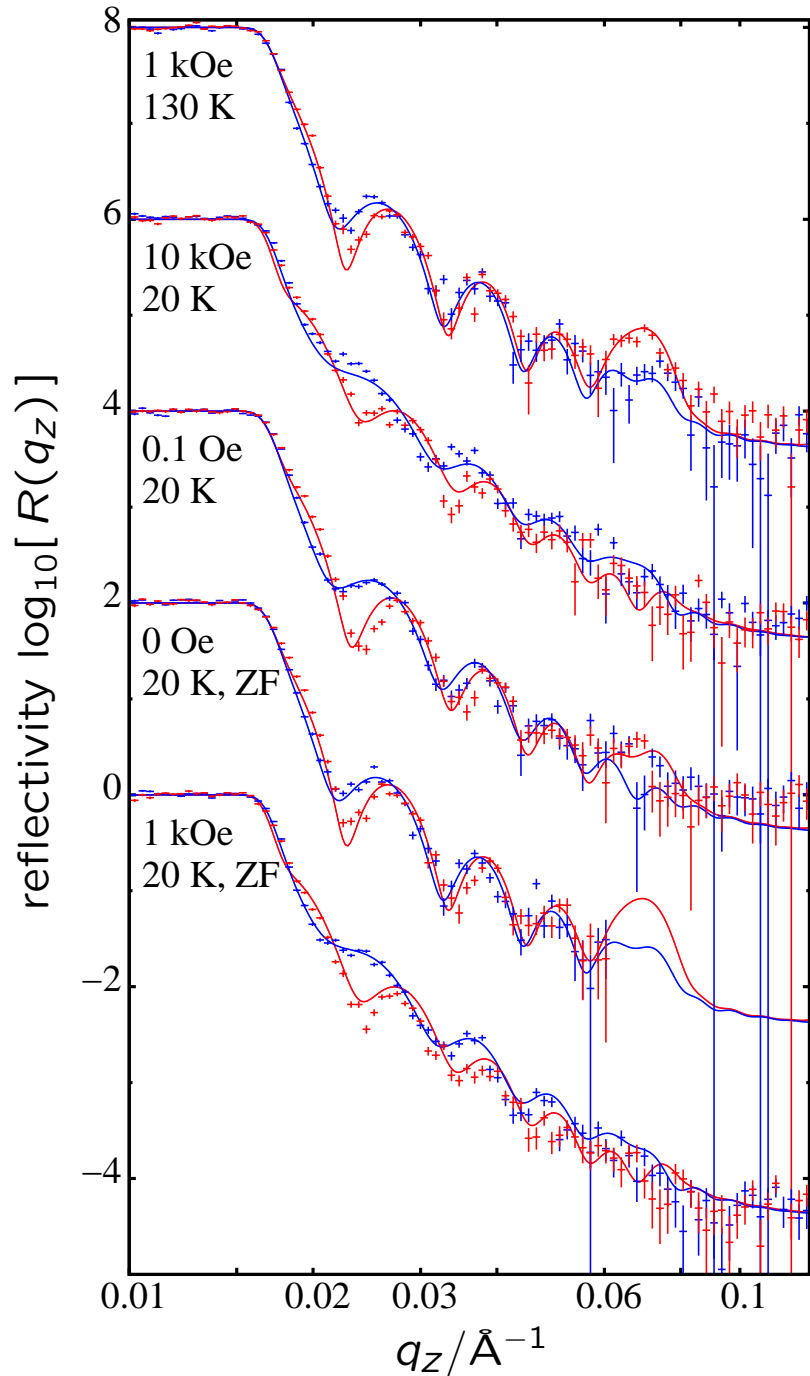
reflectometry

example: perovskite multilayer

by courtesy of C. Aruta and F. Miletto



reflectometry



PCMO
magnetism:
none
full
interfaces
none
interfaces

findings:

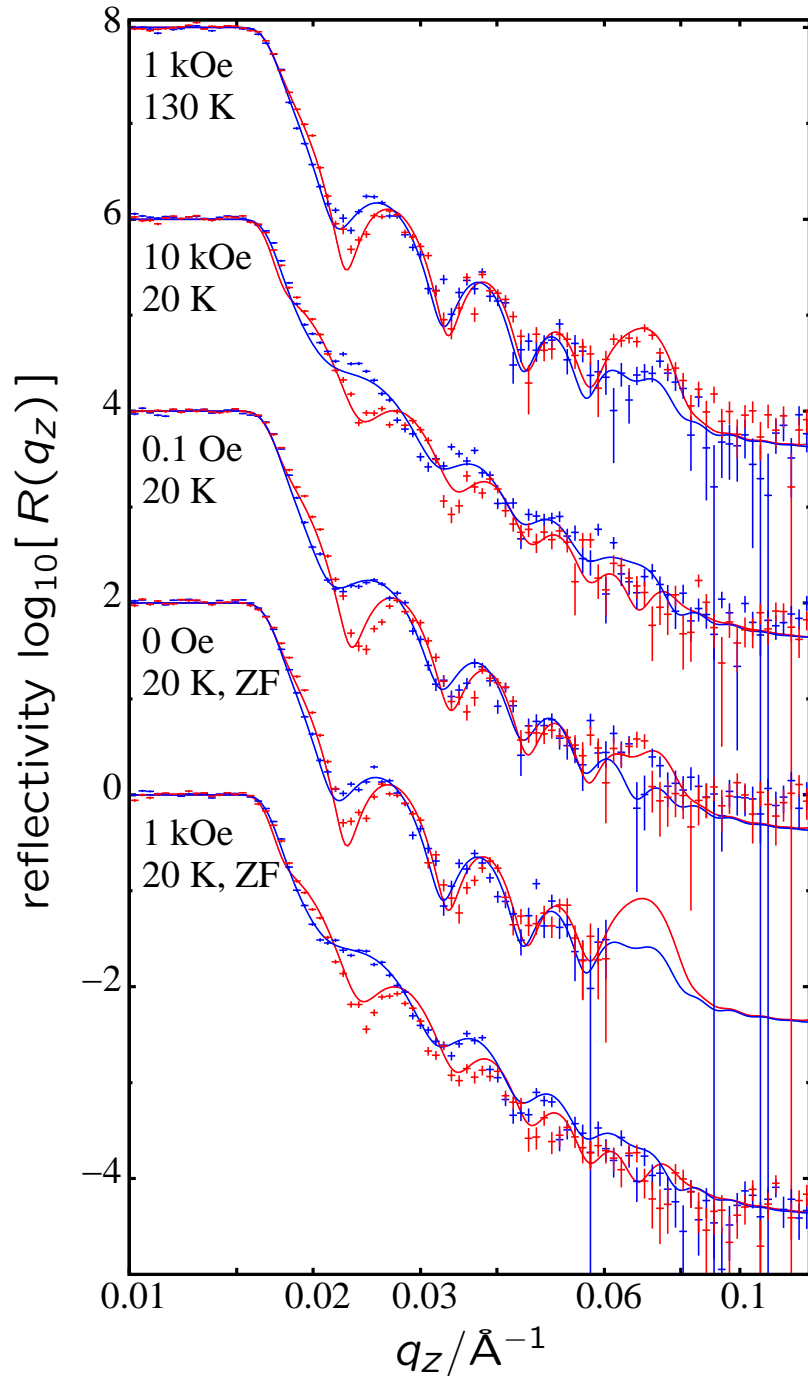
- no reduction of M within LSMO

but

- induced M in PCMO (already above T_{Curie})

to be continued ...

reflectometry



sample: $5 \times 5 \text{ mm}^2$



counting time per spin state: 12 h!



accurate screening of H
and T not possible



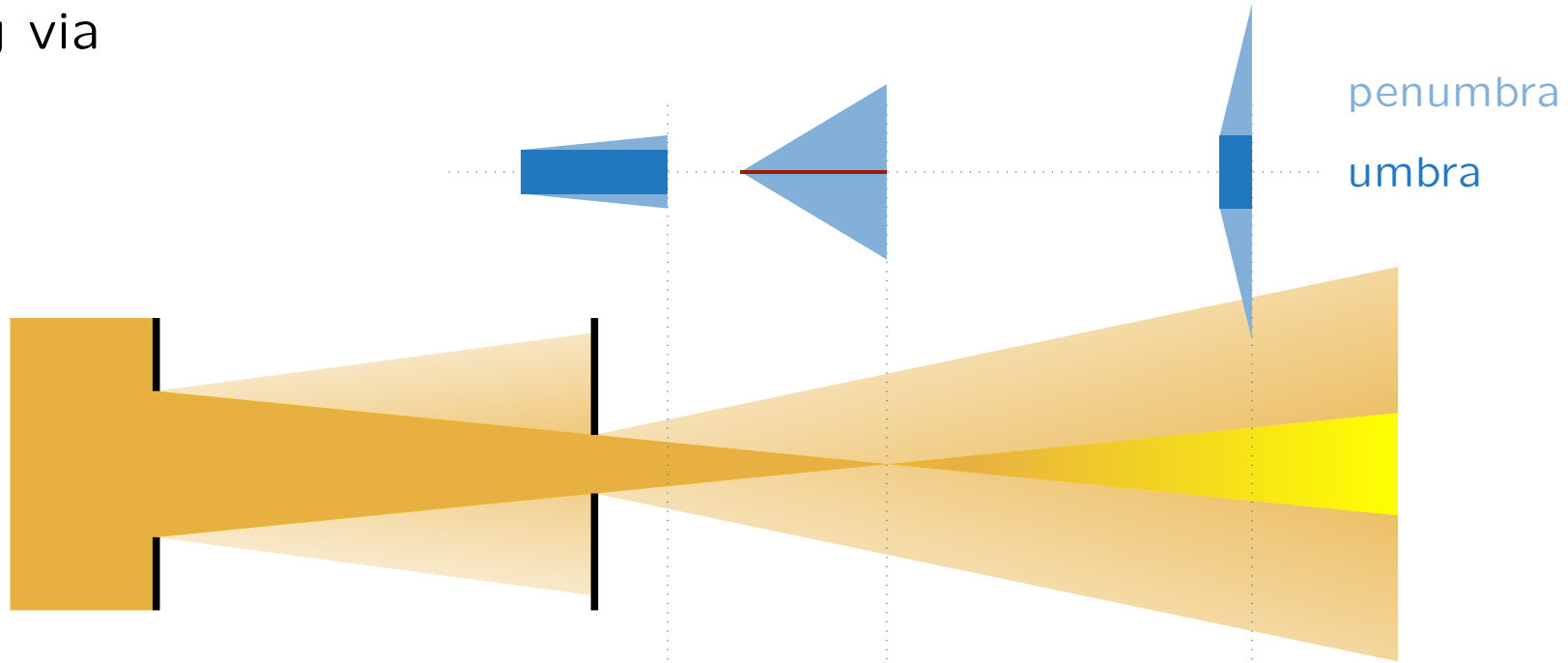
at the moment!

slit vs. focusing optics

slit vs. focusing optics

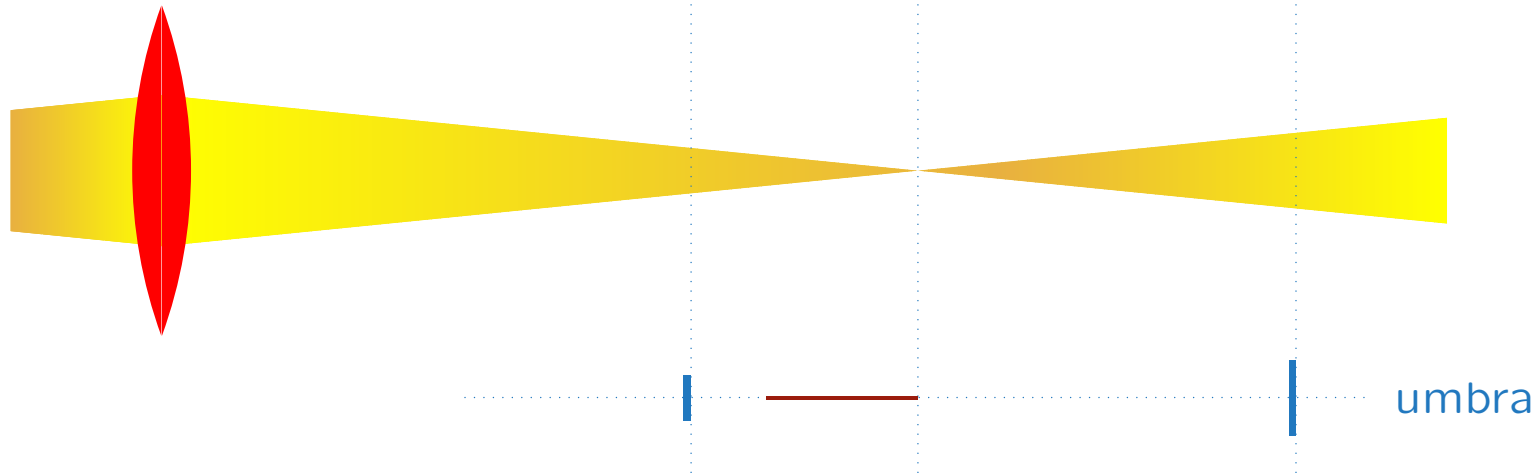
focusing via

slits



beam profile

reflective /
refractive optics

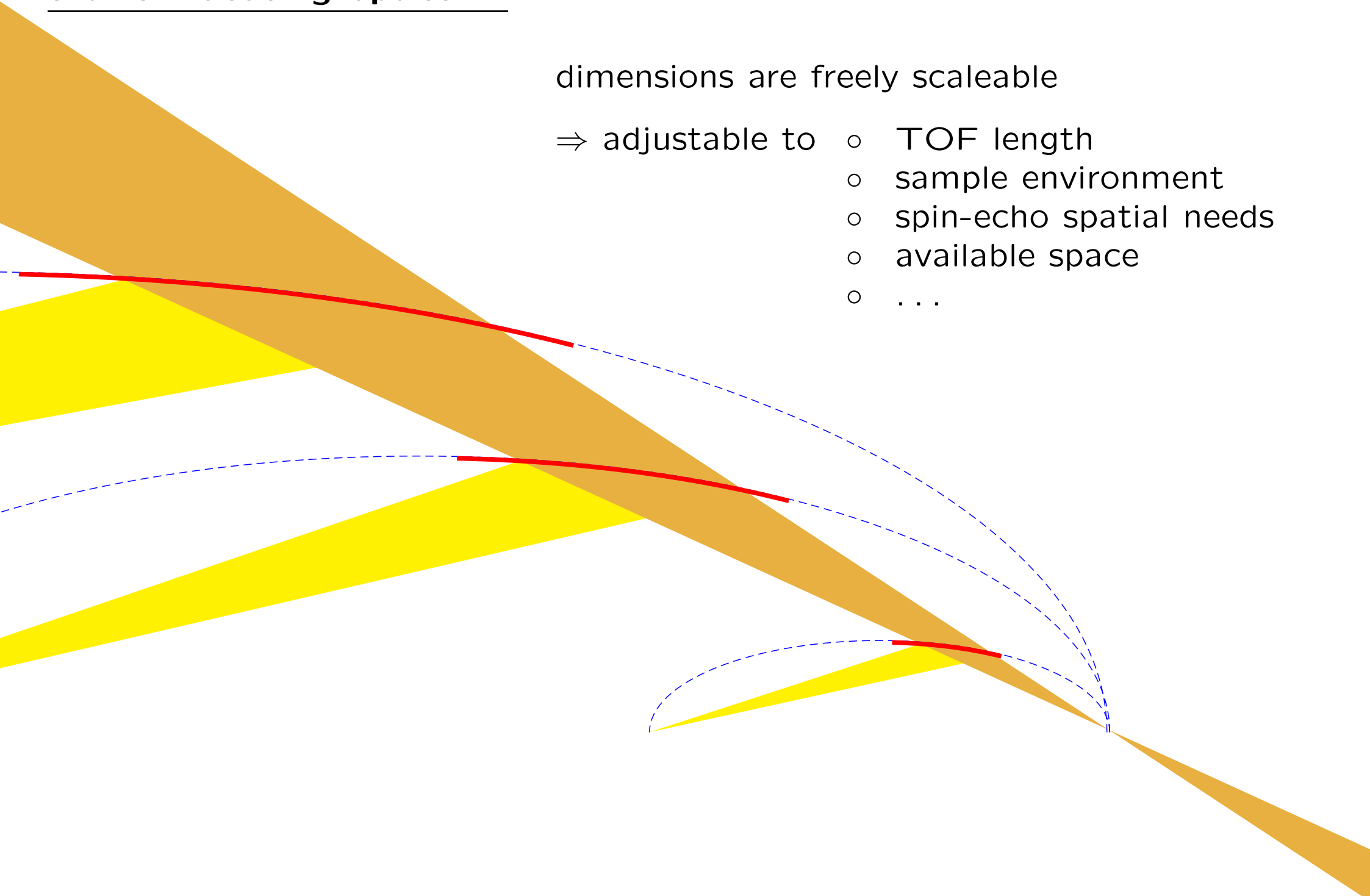


beam profile

slit vs. focusing optics

dimensions are freely scaleable

- ⇒ adjustable to
- TOF length
 - sample environment
 - spin-echo spatial needs
 - available space
 - ...

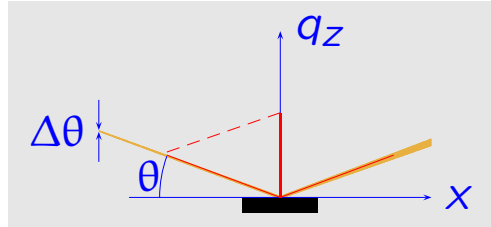


slit vs. focusing optics

focusing for high-flux specular reflectometry

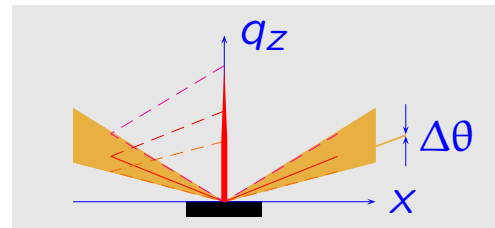
slit-defined beam:

- θ -dispersive, **or**
- λ -dispersive,
- resolution given by $\Delta\lambda$ and $\Delta\theta$



convergent beam:

- θ -dispersive **and**
- λ -dispersive,
- resolution given by $\Delta\lambda$ and detector



small samples

small samples

i.e. **samples smaller than the beam**

- e.g.
- PLD-grown samples
 - laterally structured films
 - functional devices
 - samples compatible with x-ray or magnetometry environments

projected height < 1 mm!

Ni/Ti multilayer on Si, $4 \times 3 \text{ mm}^2$

perovskite multilayer on STO, $5 \times 5 \text{ mm}^2$

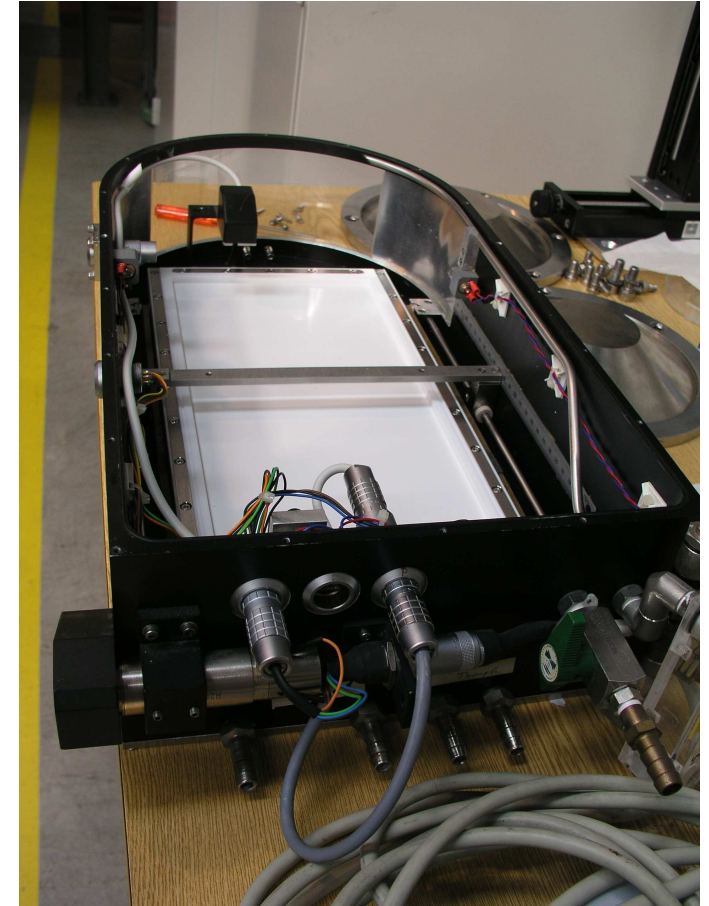


small samples

i.e. **illumination of a defined area, only**

e.g. ○ inner region within a LB-trough →

- inner region of a solid-liquid cell
- samples with electrical contacts
- partially coated substrates
- bent substrates



footprint < substrate

typical dimensions: $10 \times 10 \text{ mm}^2$ to $20 \times 40 \text{ mm}^2$

small samples

i.e. **latteraly inhomogeneous samples**

- e.g.
- structured materials
 - samples with (large) domains
 - bent surfaces →



footprint \ll substrate

typical dimensions: $0.1 \times 10 \text{ mm}^2$

\Rightarrow scanning of sample area

focusing with elliptic guides

real focusing!

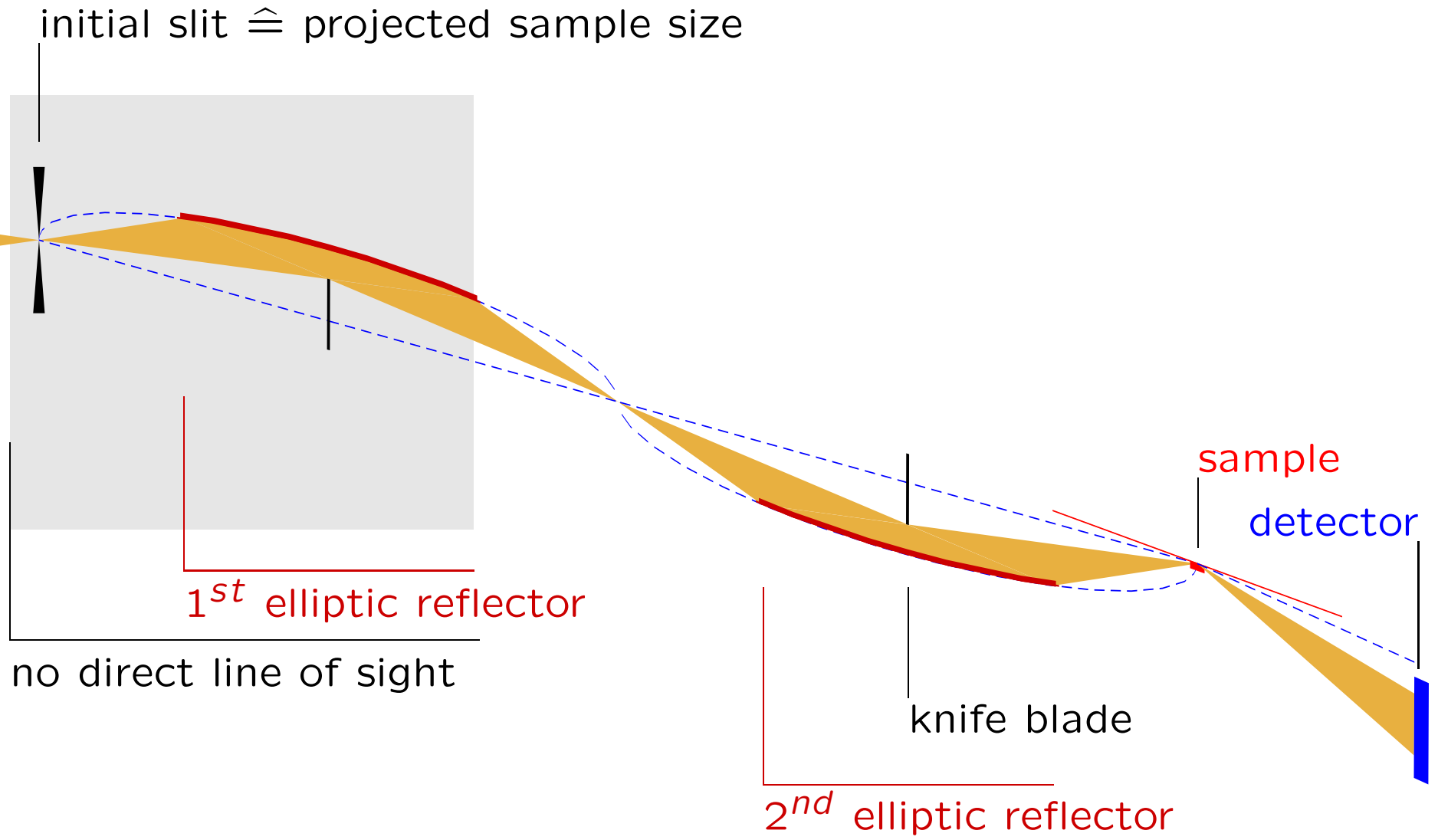
\Rightarrow pre-image \longrightarrow image

no fancy version of a ballistic guide!

focusing with elliptic guides

generic instrument layout

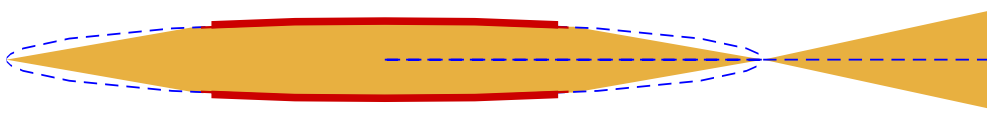
cut in the scattering plane
stretched by 10 normal to incident beam



focusing with elliptic guides

why only one branch of an ellipse?

- no structured $I(\theta, z)$

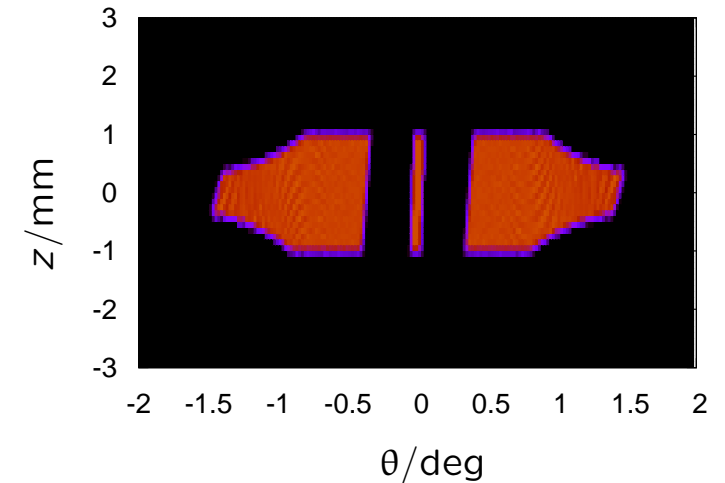


- one branch can cover $\Delta\theta$

why two subsequent elliptic guides?

- convenient beam manipulation
- guide dimensions not too large
- correction for coma aberration!

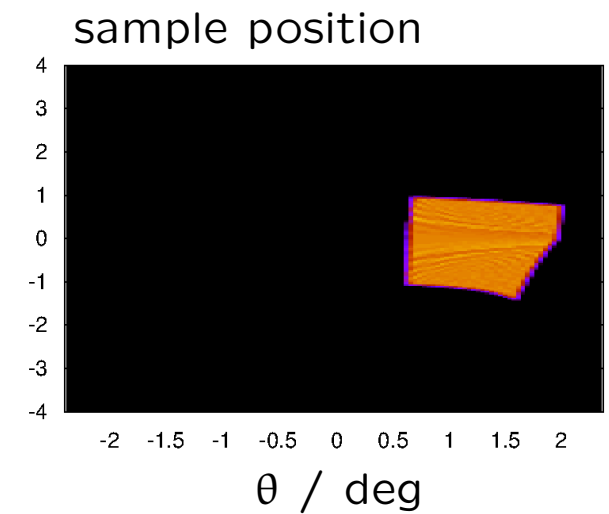
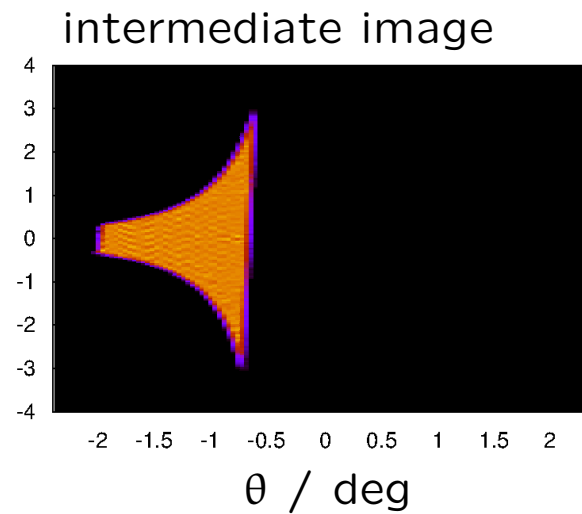
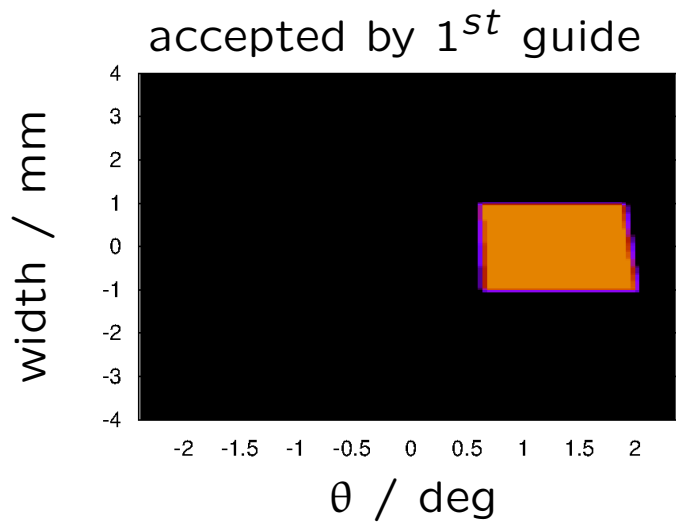
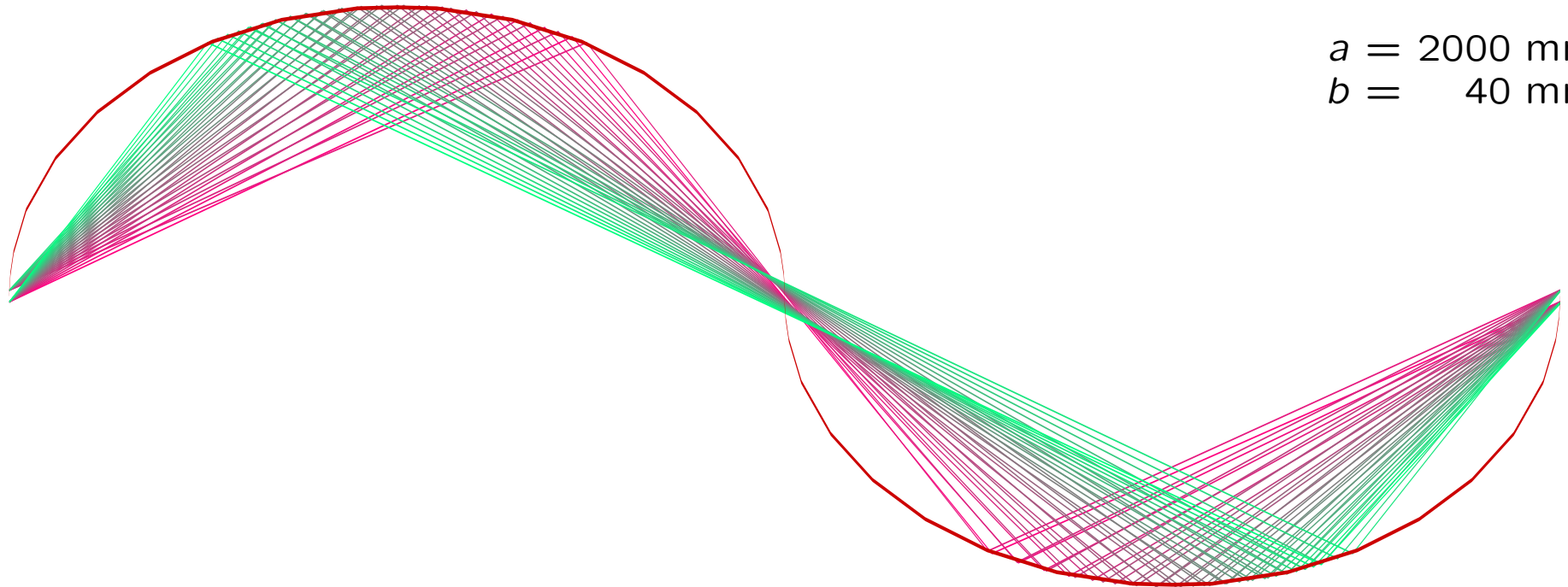
$I(\theta, z)$ map



focusing with elliptic guides

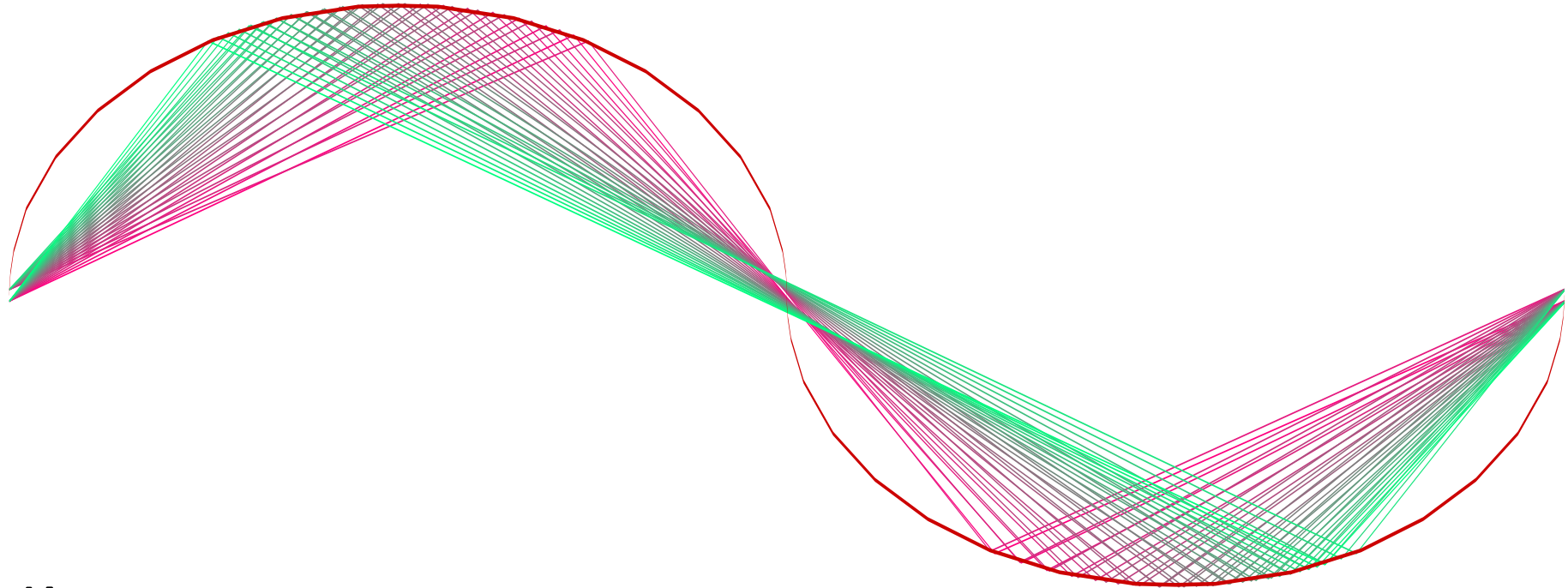
coma aberration — and its correction

$a = 2000$ mm
 $b = 40$ mm



focusing with elliptic guides

coma aberration — and its correction



limitations:

- finite length of the guides
- non-perfect coating

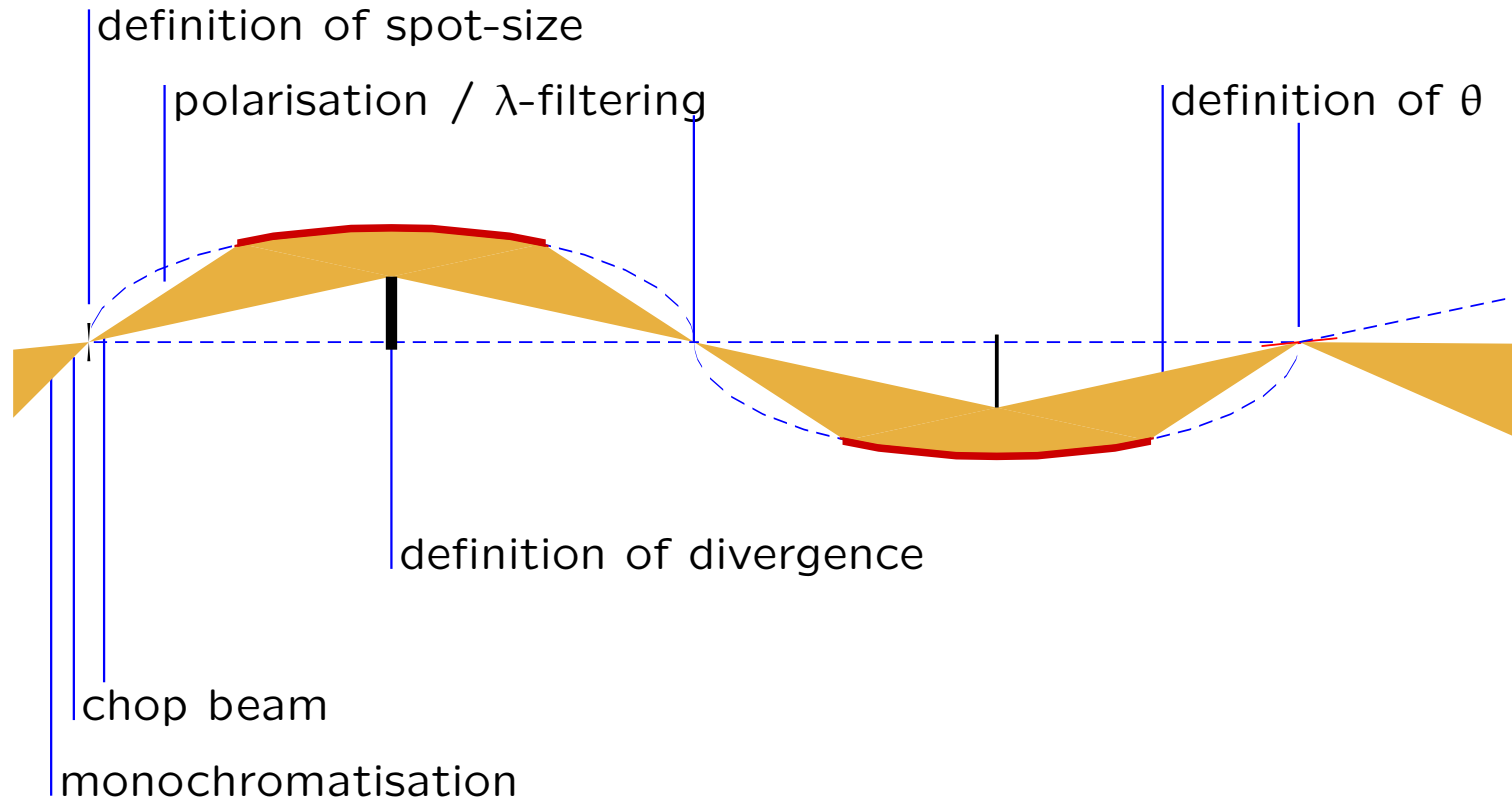
opportunities:

- use aberration to reduce beam spot or divergence at the sample

focusing with elliptic guides

operation modes for TOF:

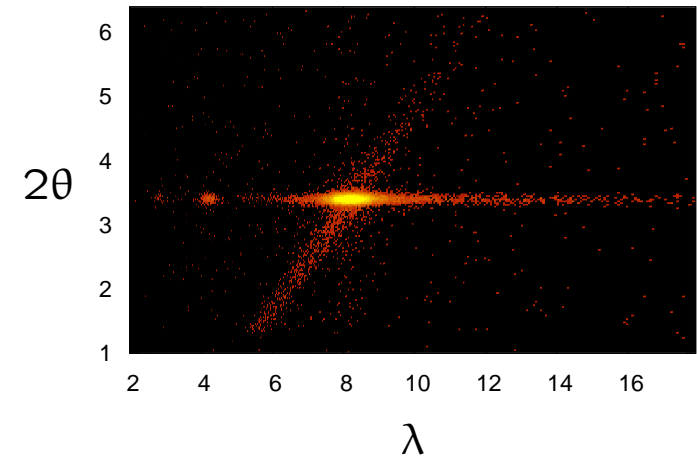
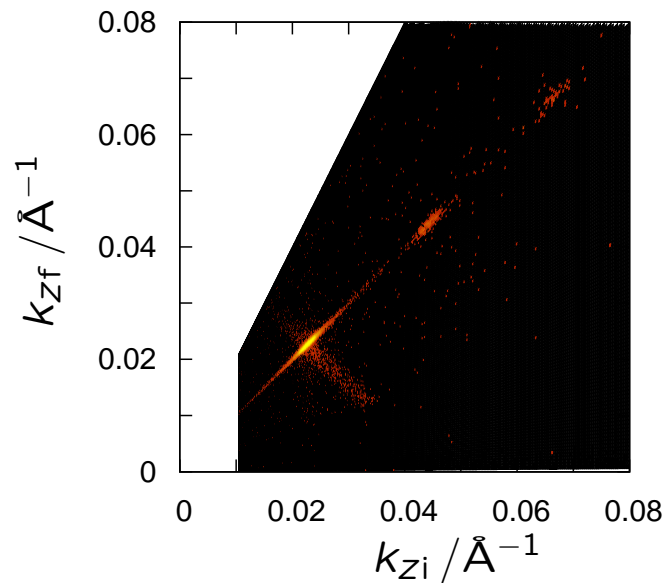
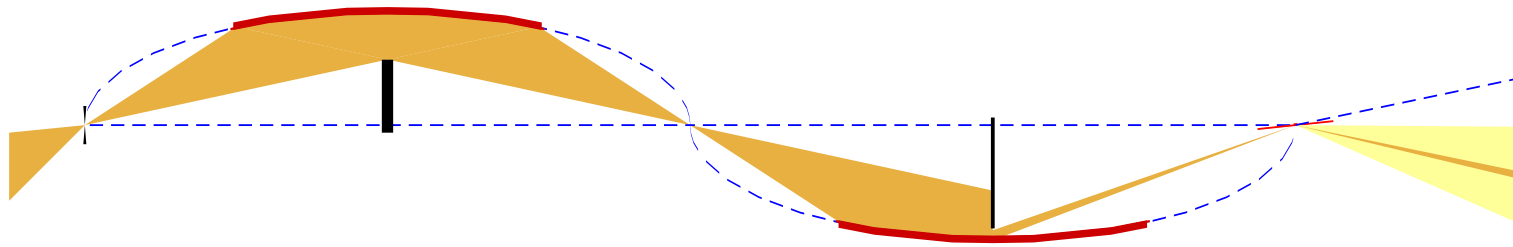
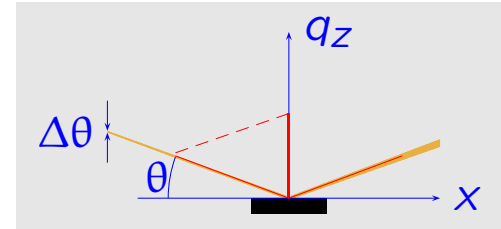
(non-TOF operation is also possible!)



focusing with elliptic guides

mode: almost conventional

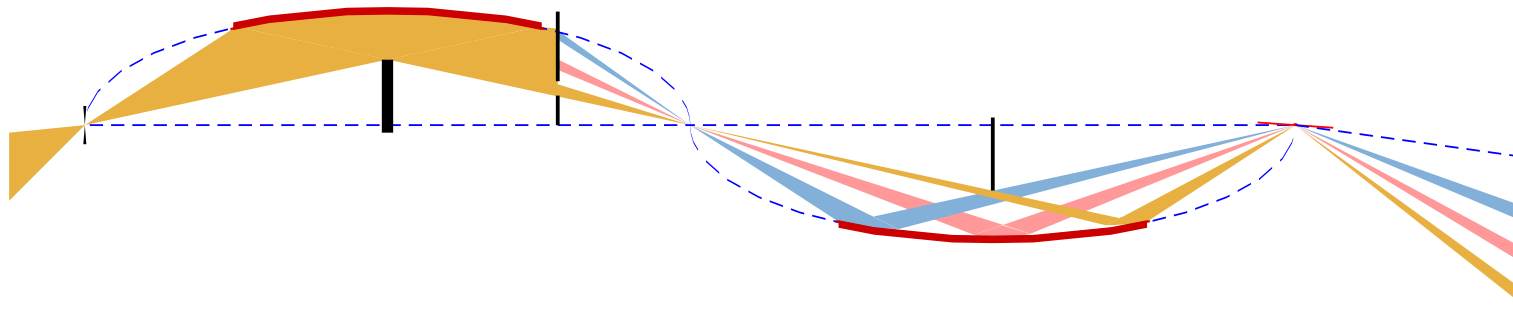
- beam is still convergent
- off-specular measurements are feasible



focusing with elliptic guides

mode: wide q -range

- vary θ with fixed sample position
- shift diaphragm (chopper) between pulses



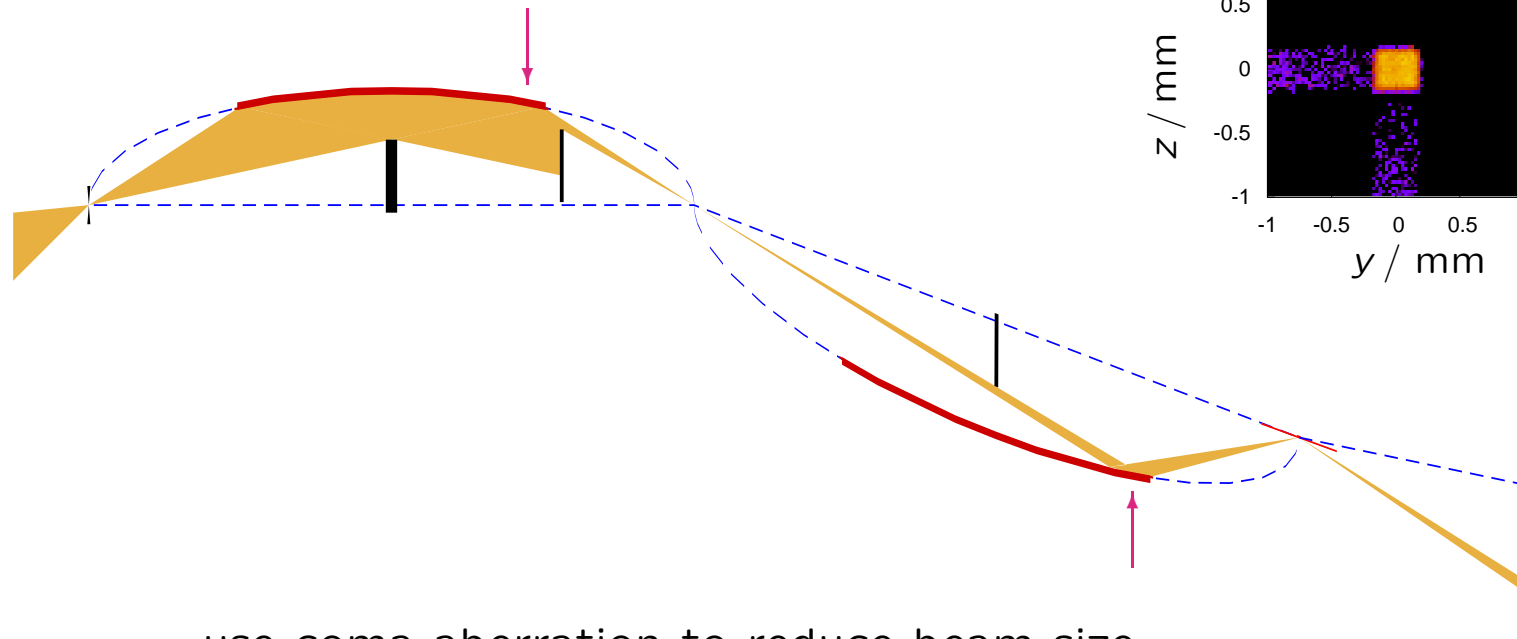
- suited for liquid surfaces

focusing with elliptic guides

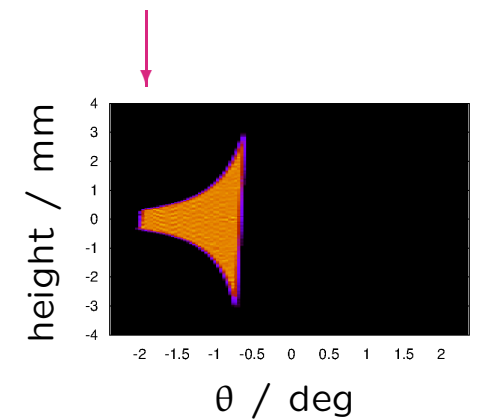
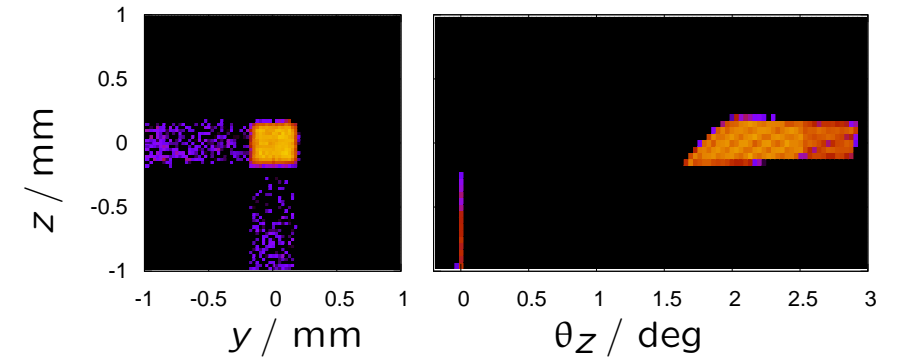
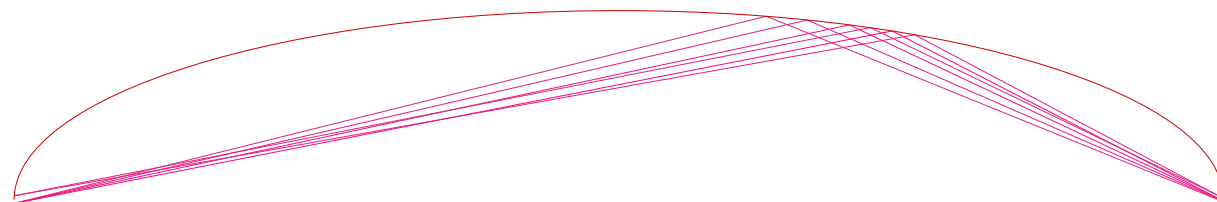
mode: small spot size

- uses focusing due to coma aberration
- scanning mode possible

$I(y, z)$ and $I(z, \theta_z)$ at the sample
for a $1 \times 1 \text{ mm}^2$ entrance slit



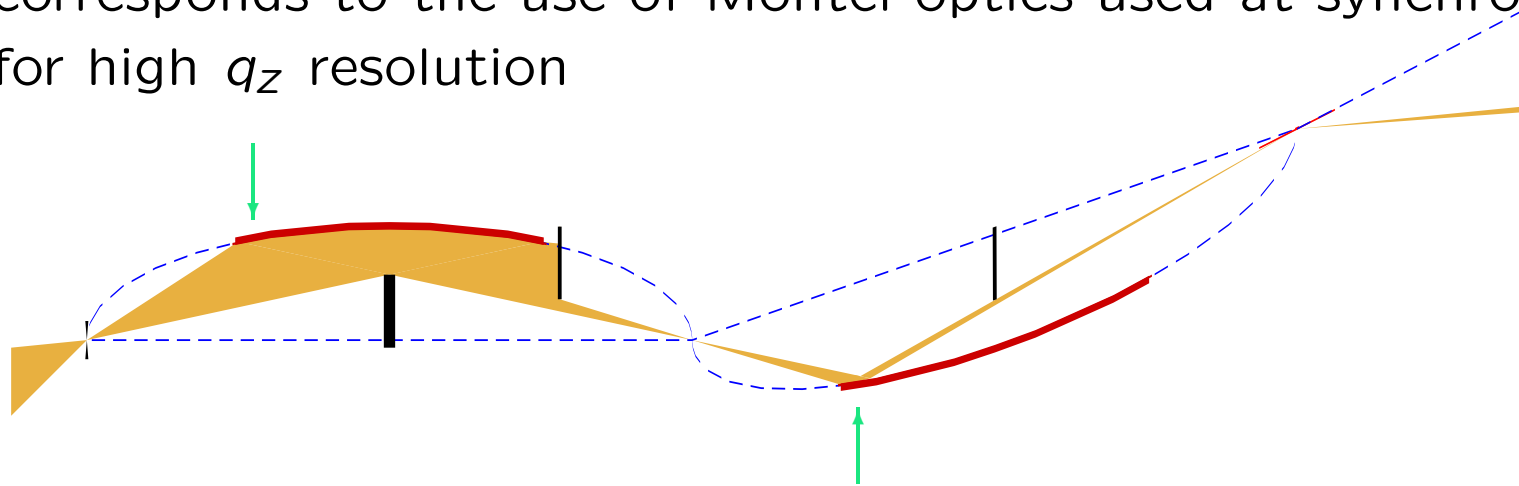
use coma aberration to reduce beam size



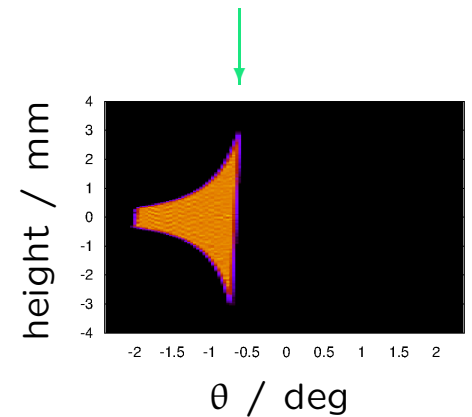
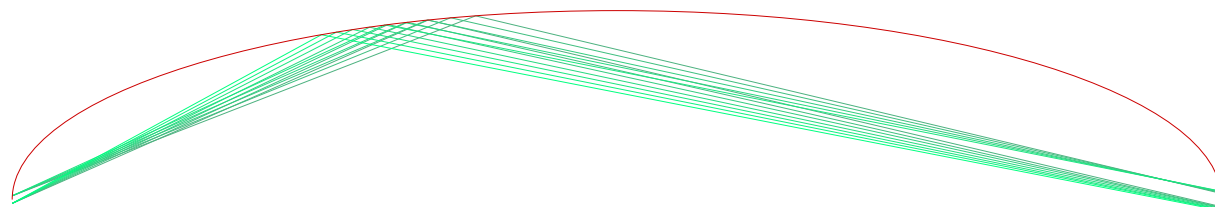
focusing with elliptic guides

mode: low-divergent beam

- uses defocusing due to coma aberration
- corresponds to the use of Montel optics used at synchrotrons
- for high q_z resolution



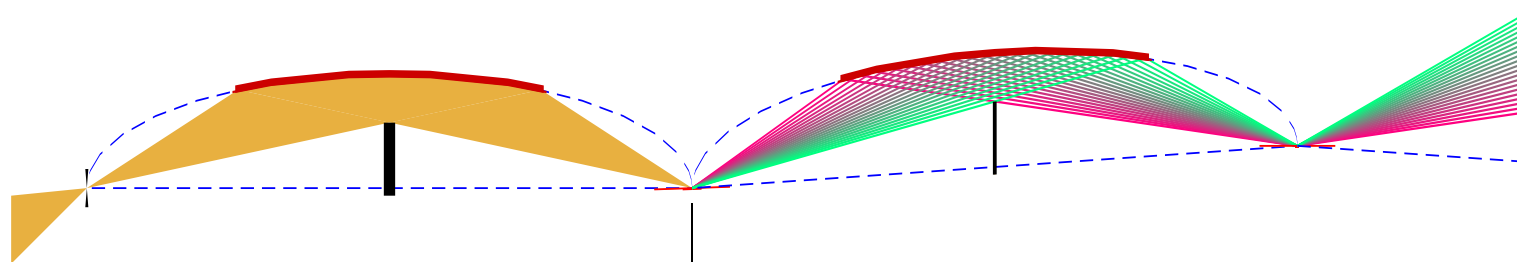
use coma aberration to reduce divergence



focusing with elliptic guides

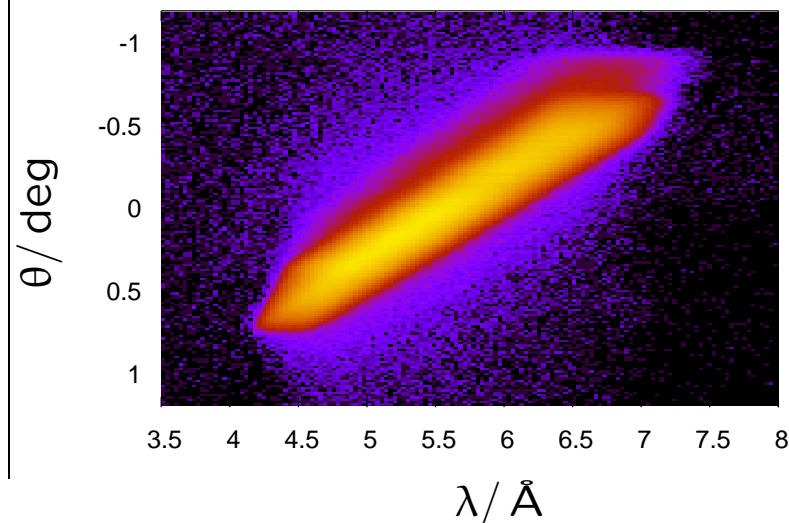
mode: angle/energy encoding

- use a ml-monochromator at the intermediate image
- spectral analysis of the beam: λ / θ encoding



- large λ on small θ
 \Rightarrow wide q_z -range

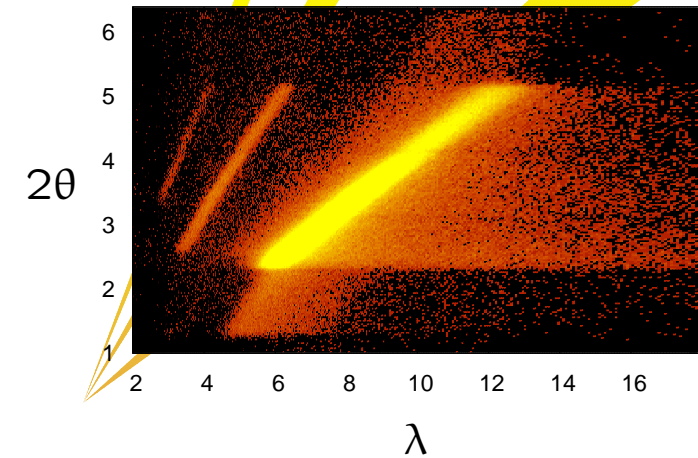
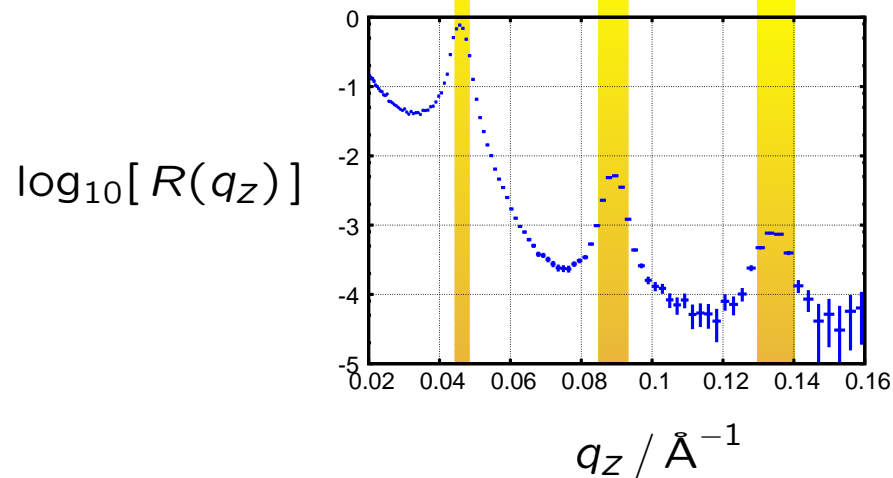
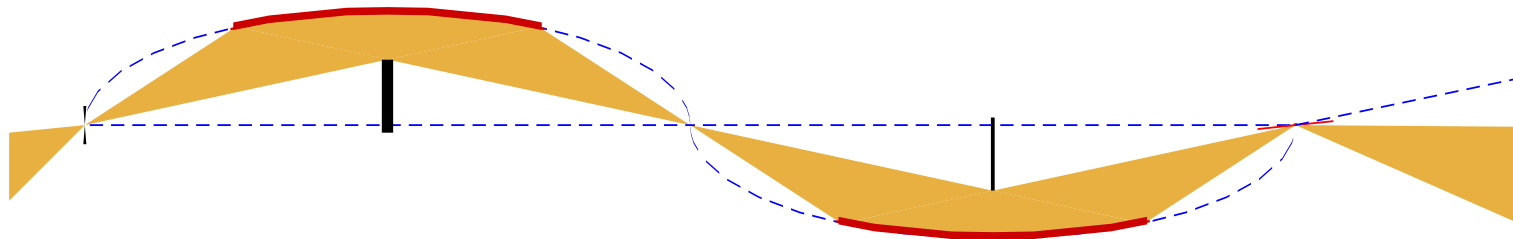
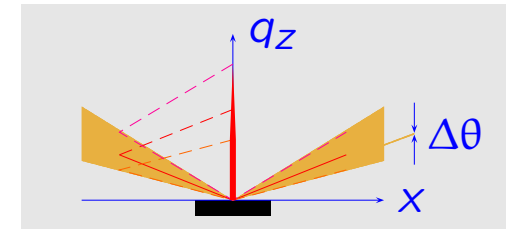
$\log_{10} [I(\lambda, \theta)]$ after ml monochromator



focusing with elliptic guides

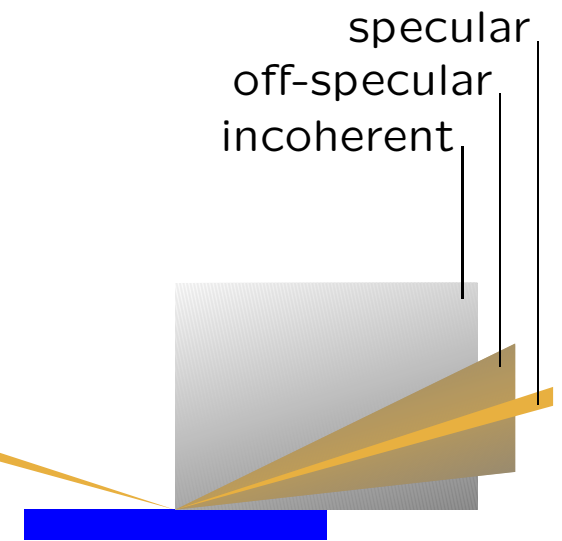
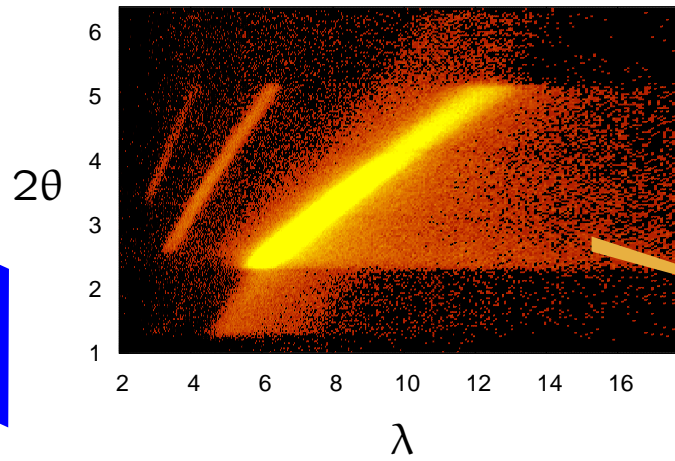
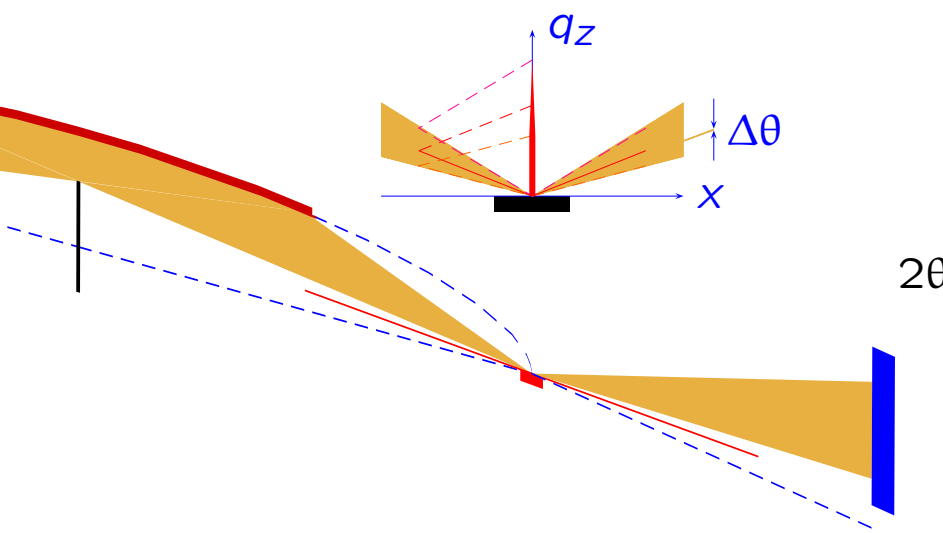
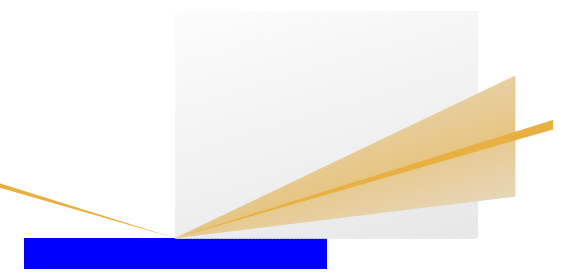
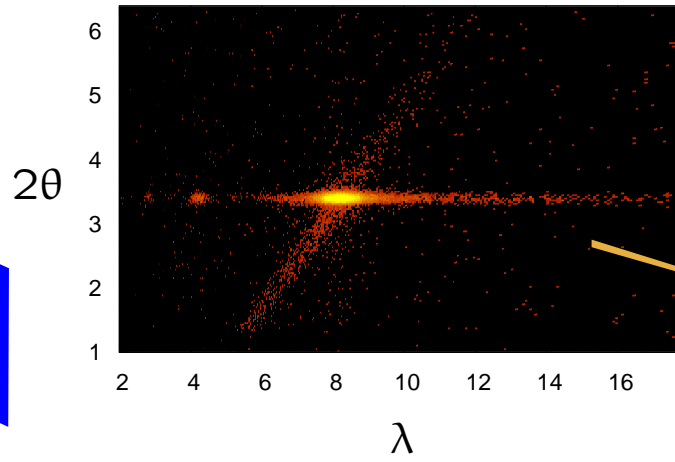
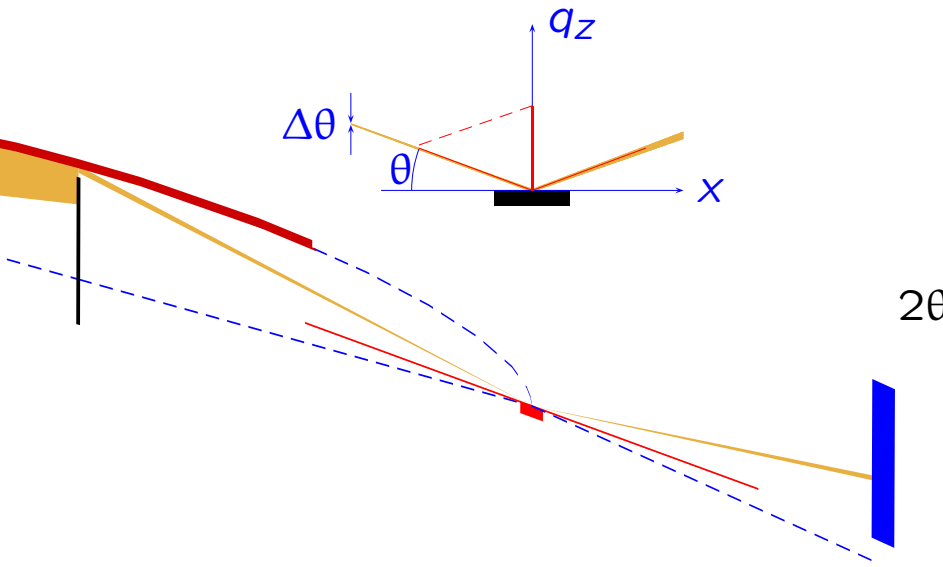
mode: high-intensity specular reflectivity

- energy- and angle-dispersive \Rightarrow gain > 10
- for fast scanning ($T, H, E \dots$)
- or if off-specular scattering is no *problem*



focusing with elliptic guides

high-intensity specular reflectivity vs. almost conventional



specular
off-specular
incoherent

realisation

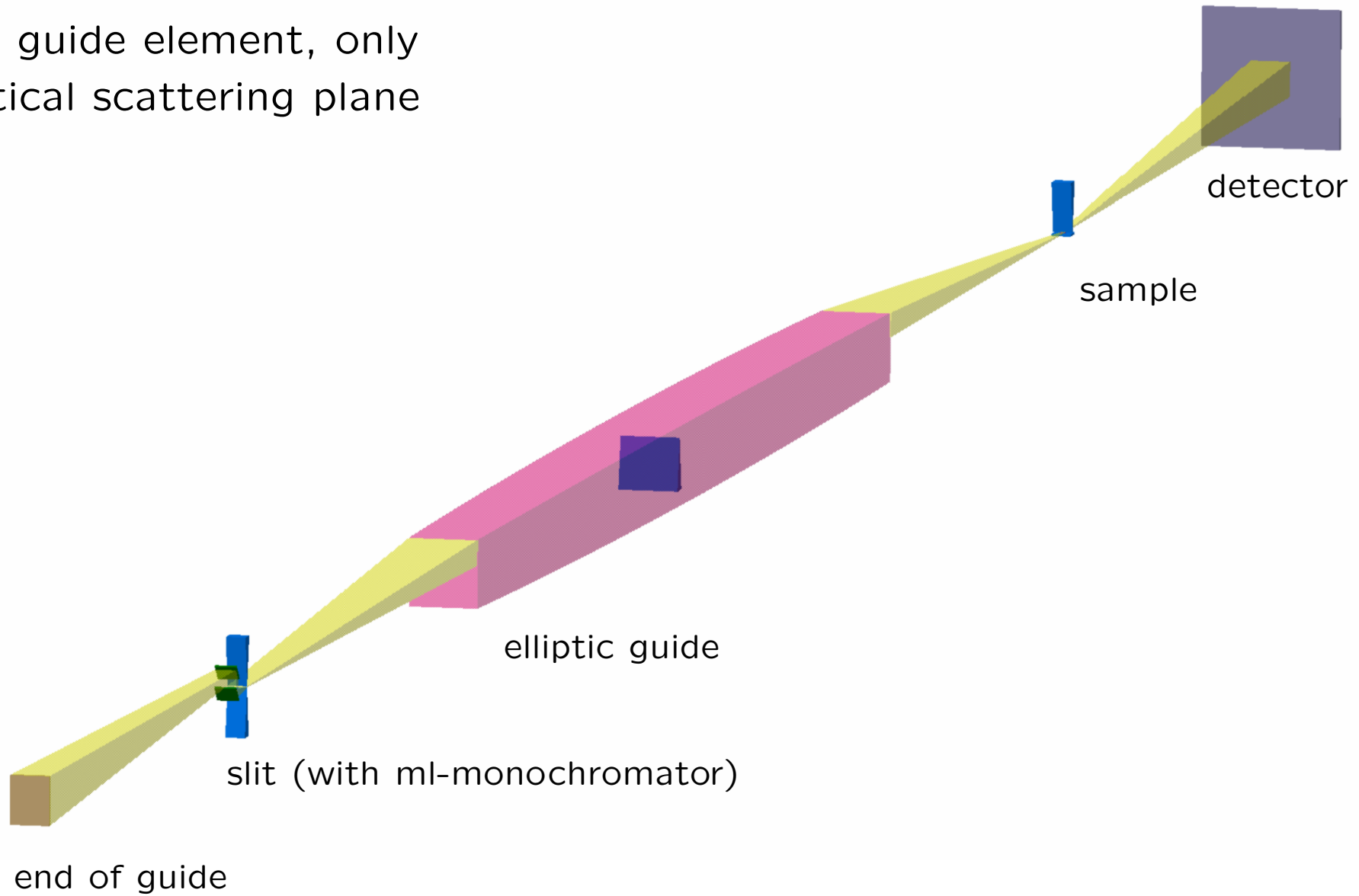
add-on for Amor

prototype on BOA

concept for the ESS

realisation: add-on for Amor

one guide element, only vertical scattering plane



realisation: add-on for Amor

Amor, conventional TOF set-up

8 m granite block

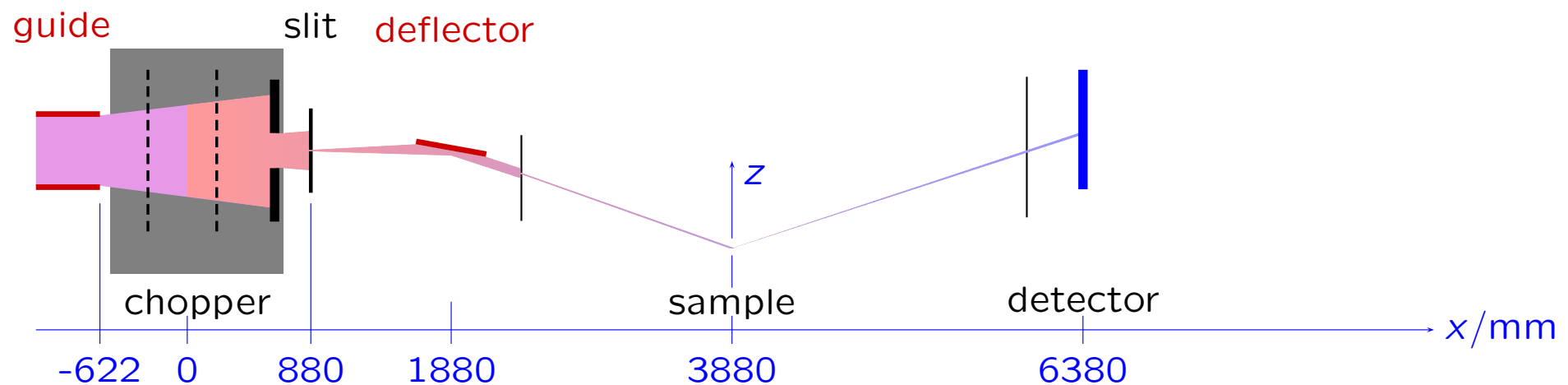
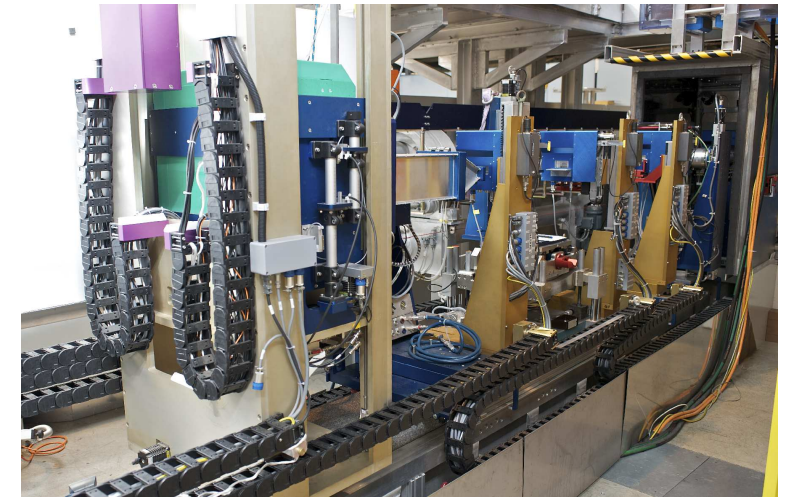
maximum length chopper to detector = 10 m

$2\theta \in [-3^\circ, 12^\circ]$

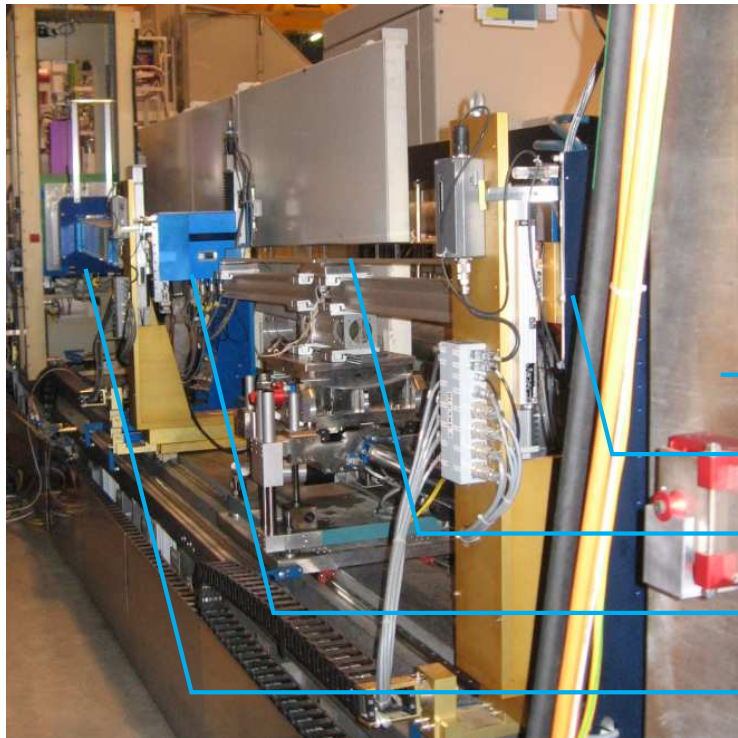
$\lambda \in [2 \text{ \AA}, 18 \text{ \AA}]$

vertical scattering plane

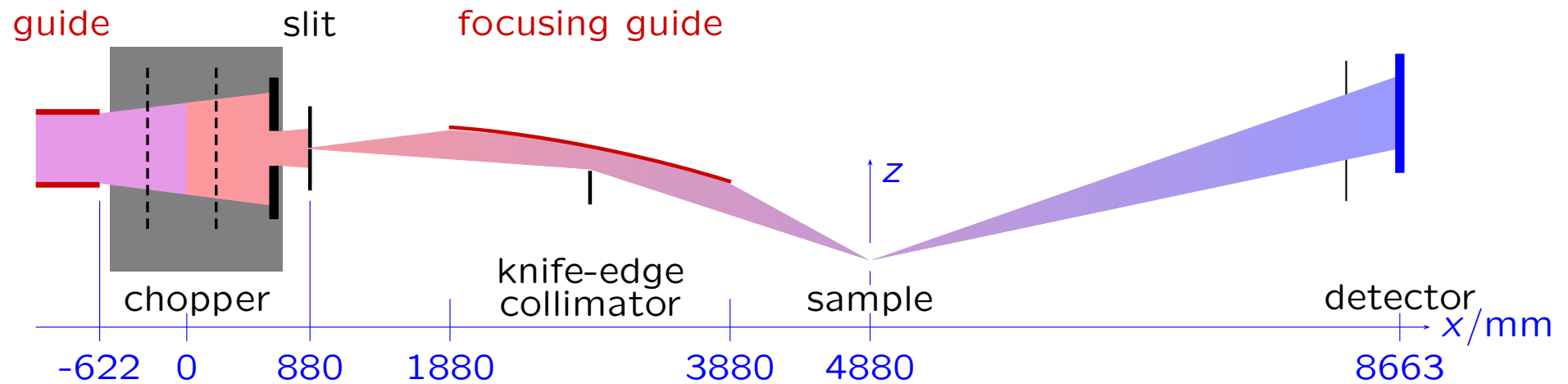
detectors: ^3He single and area ($180 \times 180 \text{ mm}^2$)



realisation: add-on for Amor

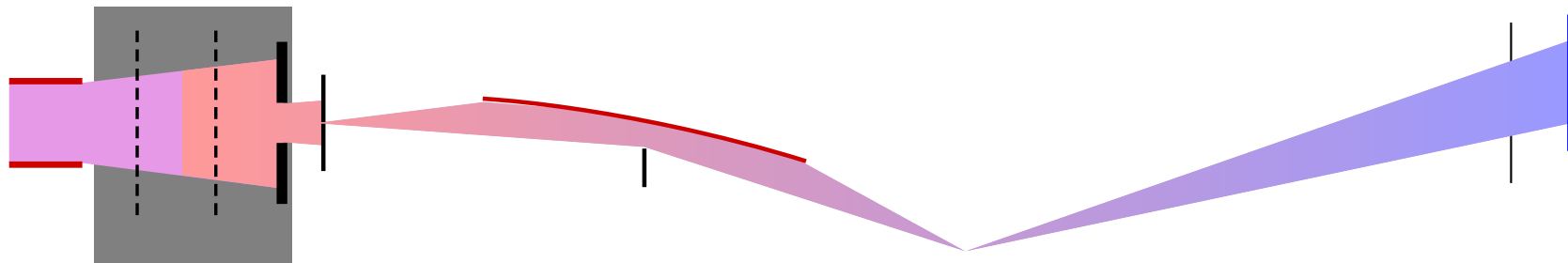
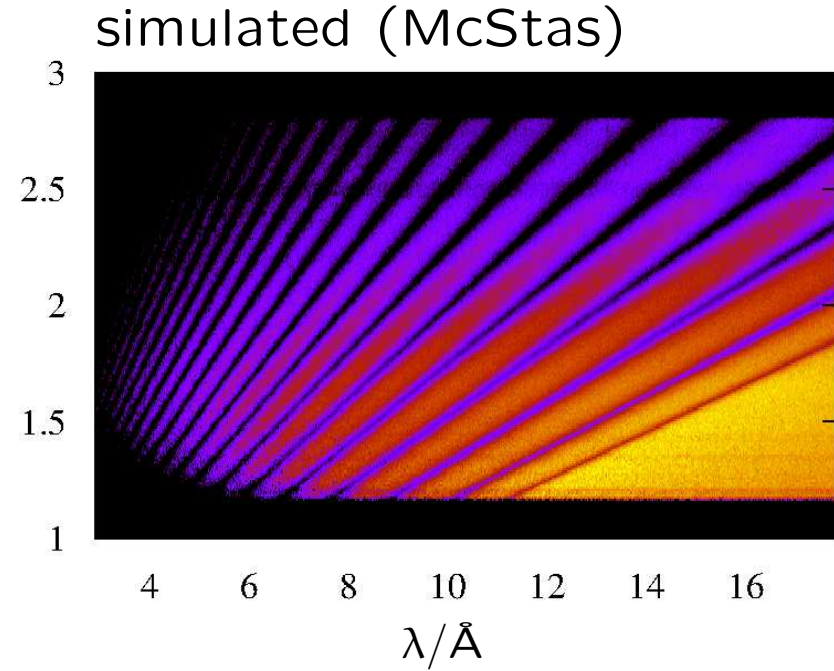
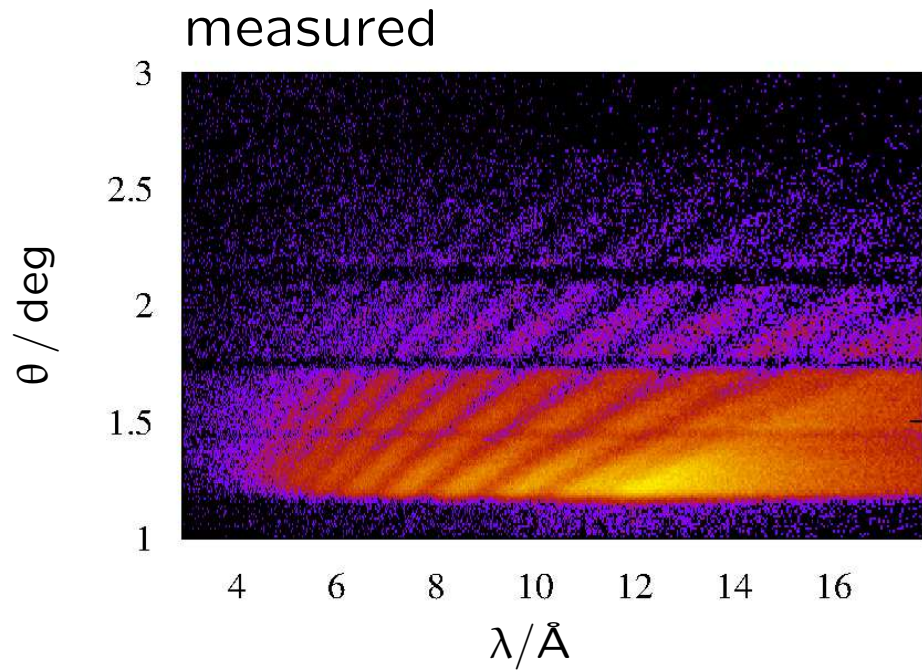


- chopper housing
- 1st slit
- elliptic reflector (SwissNeutronics)
- sample (hidden by diaphragm)
- detector



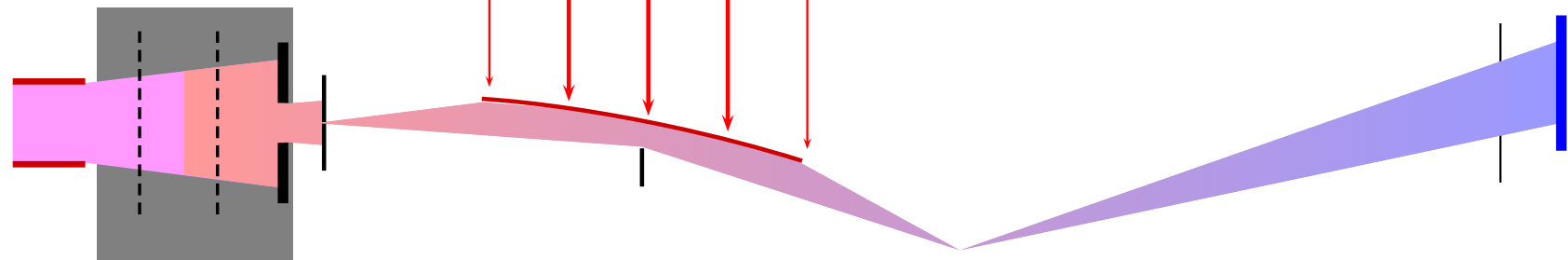
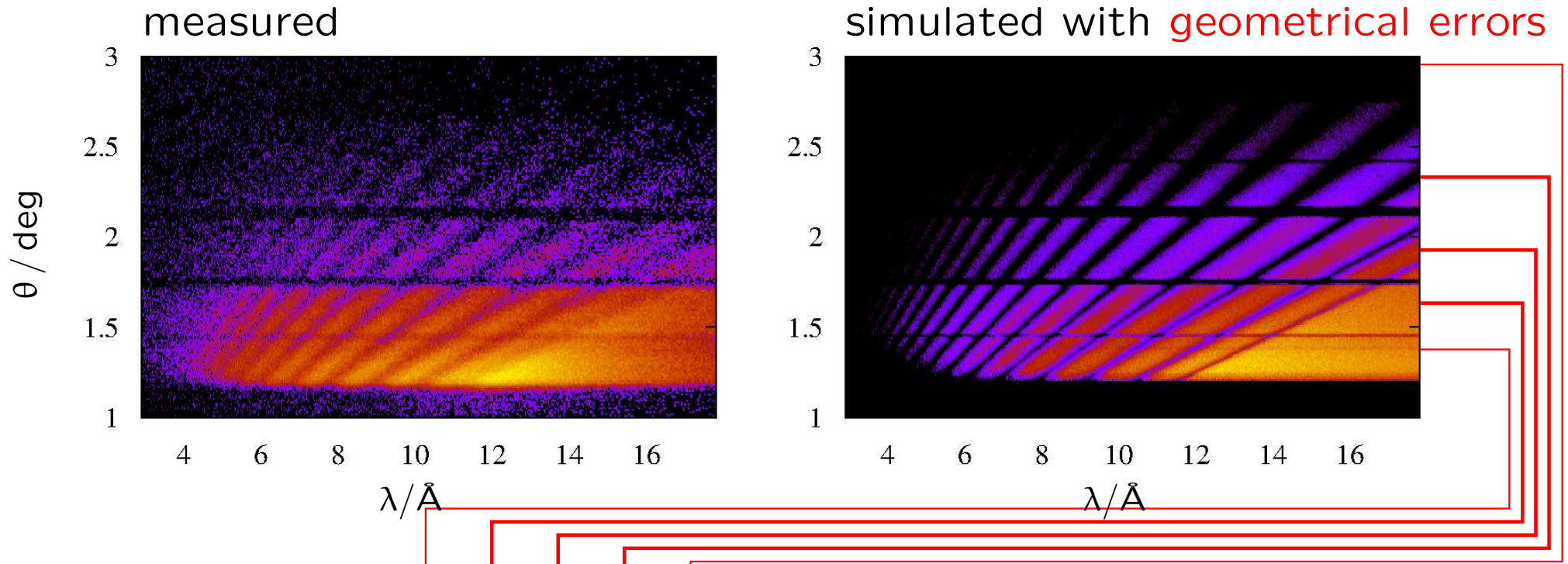
realisation: add-on for Amor

measurements: 1000 Å Ni film on glass, $9 \times 9 \text{ mm}^2$



realisation: add-on for Amor

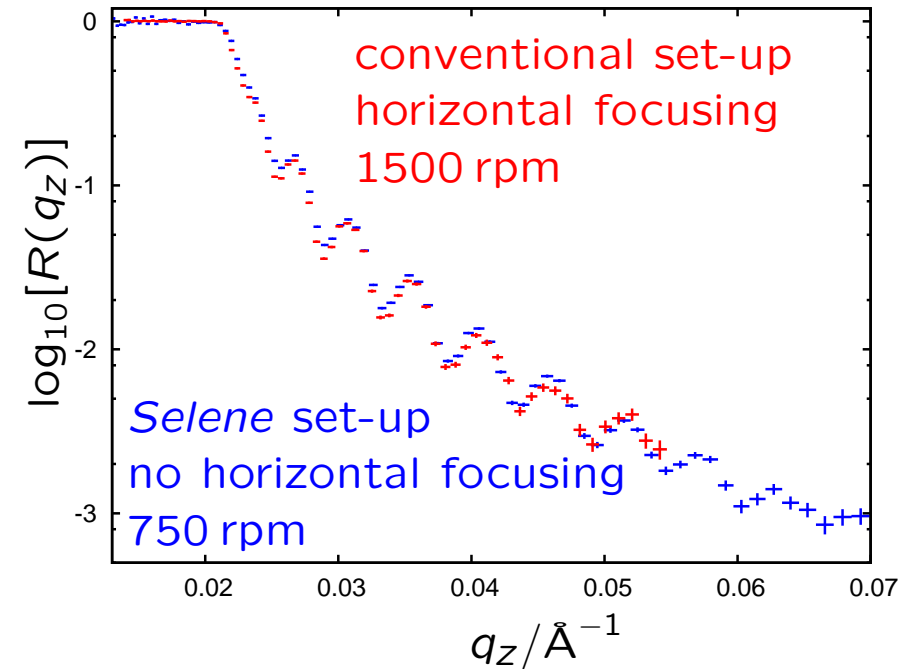
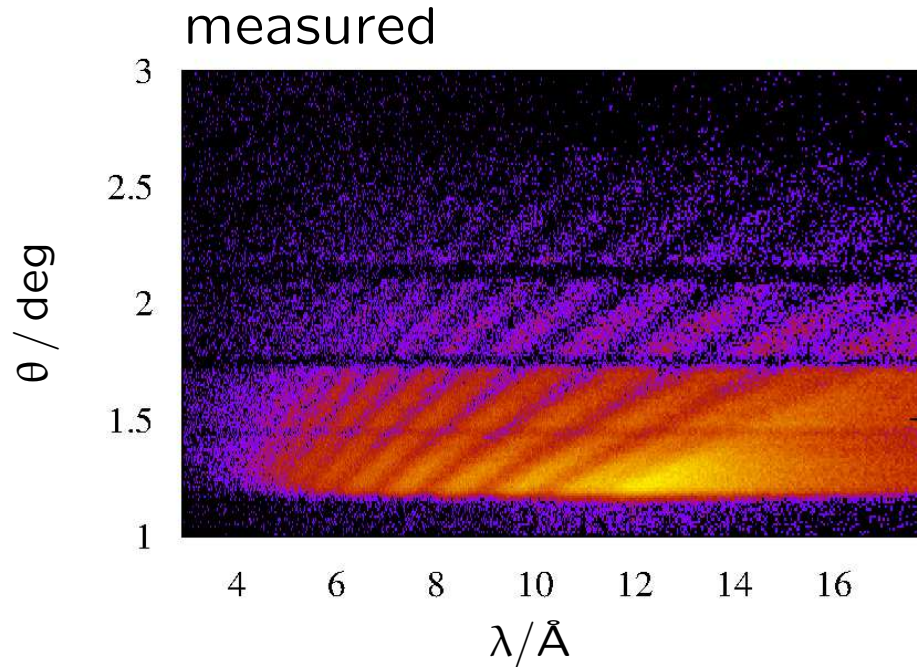
measurements: 1000 Å Ni film on glass, $9 \times 9 \text{ mm}^2$



4 guide elements à 500 mm

realisation: add-on for Amor

measurements: 1000 Å Ni film on glass, $9 \times 9 \text{ mm}^2$



measurement time:

conventional	5 h
<i>Selene</i>	<u>45 min</u>

gain-factor 6.7

realisation: add-on for Amor

$[\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3 / \text{SrTiO}_3]_4 / \text{NGO}$

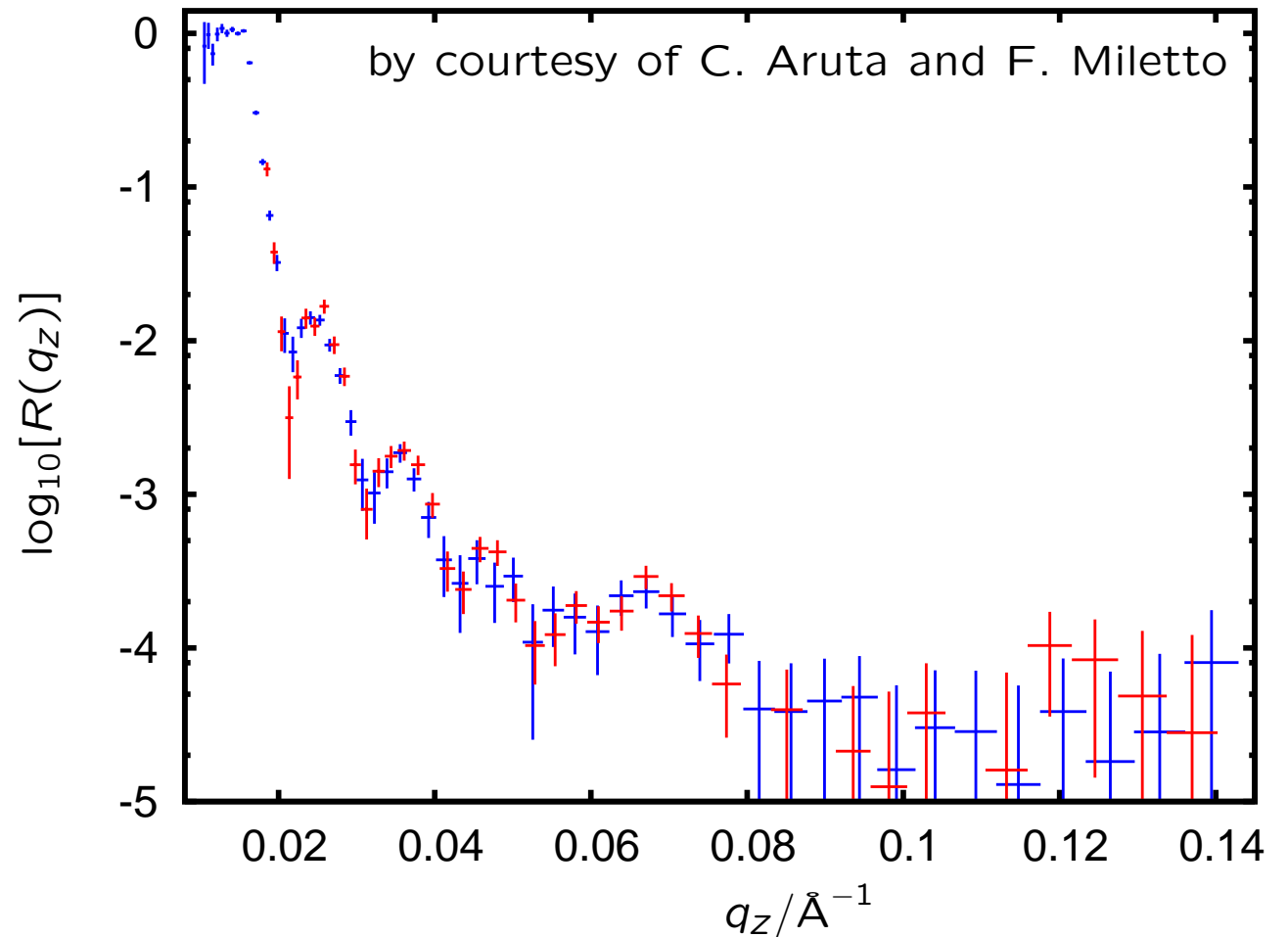
$5 \times 5 \text{ mm}^2$

- no focusing in sample plane
- TOF mode, $\lambda \in [2 \dots 18 \text{ \AA}]$
- measurement time:

conventional	6.5 h
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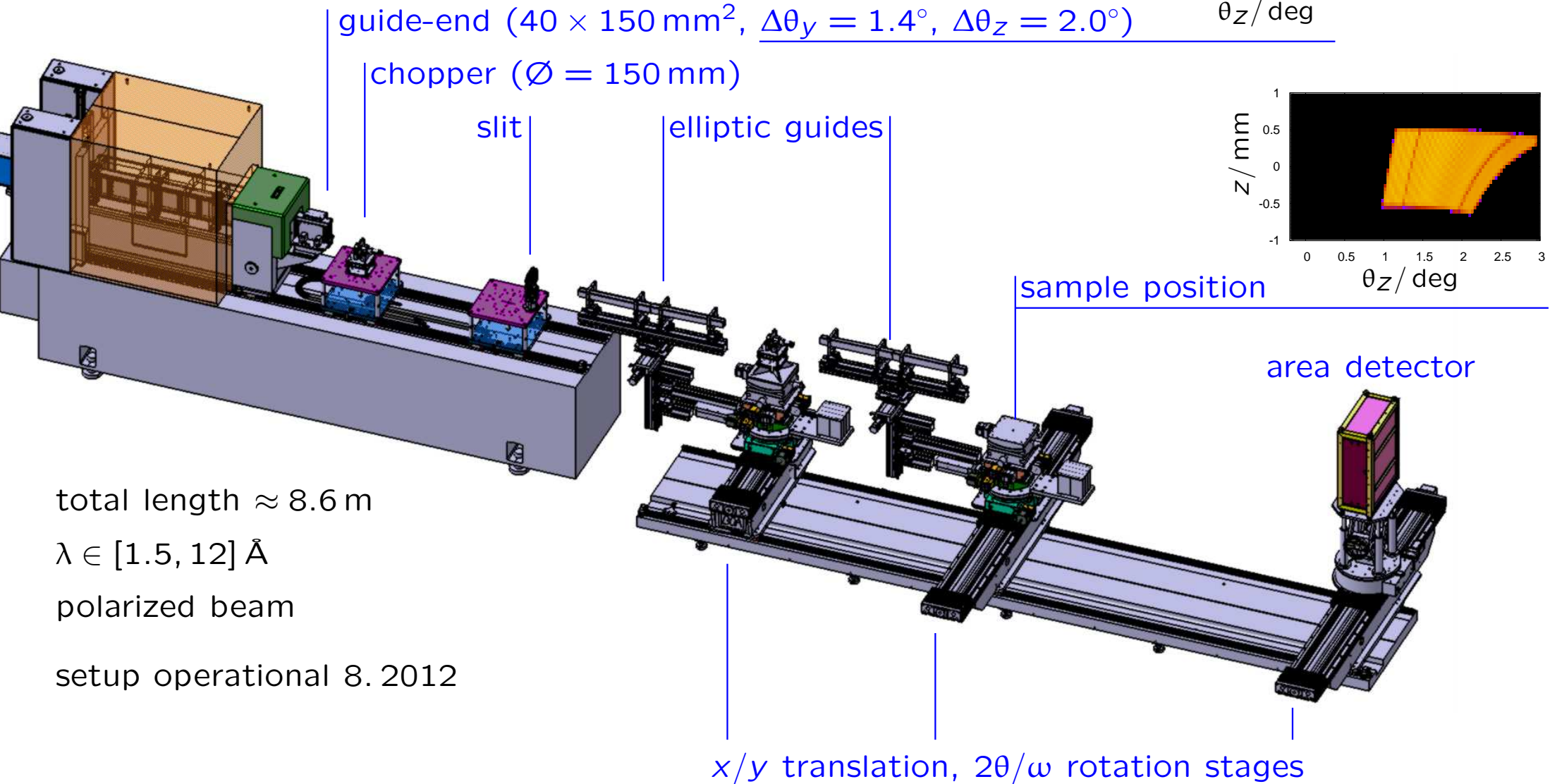
<i>Selene</i>	45 min
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gain-factor	8.3
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realisation: prototype on BOA

BOA is a test beam line at SINQ, PSI



total length $\approx 8.6 \text{ m}$

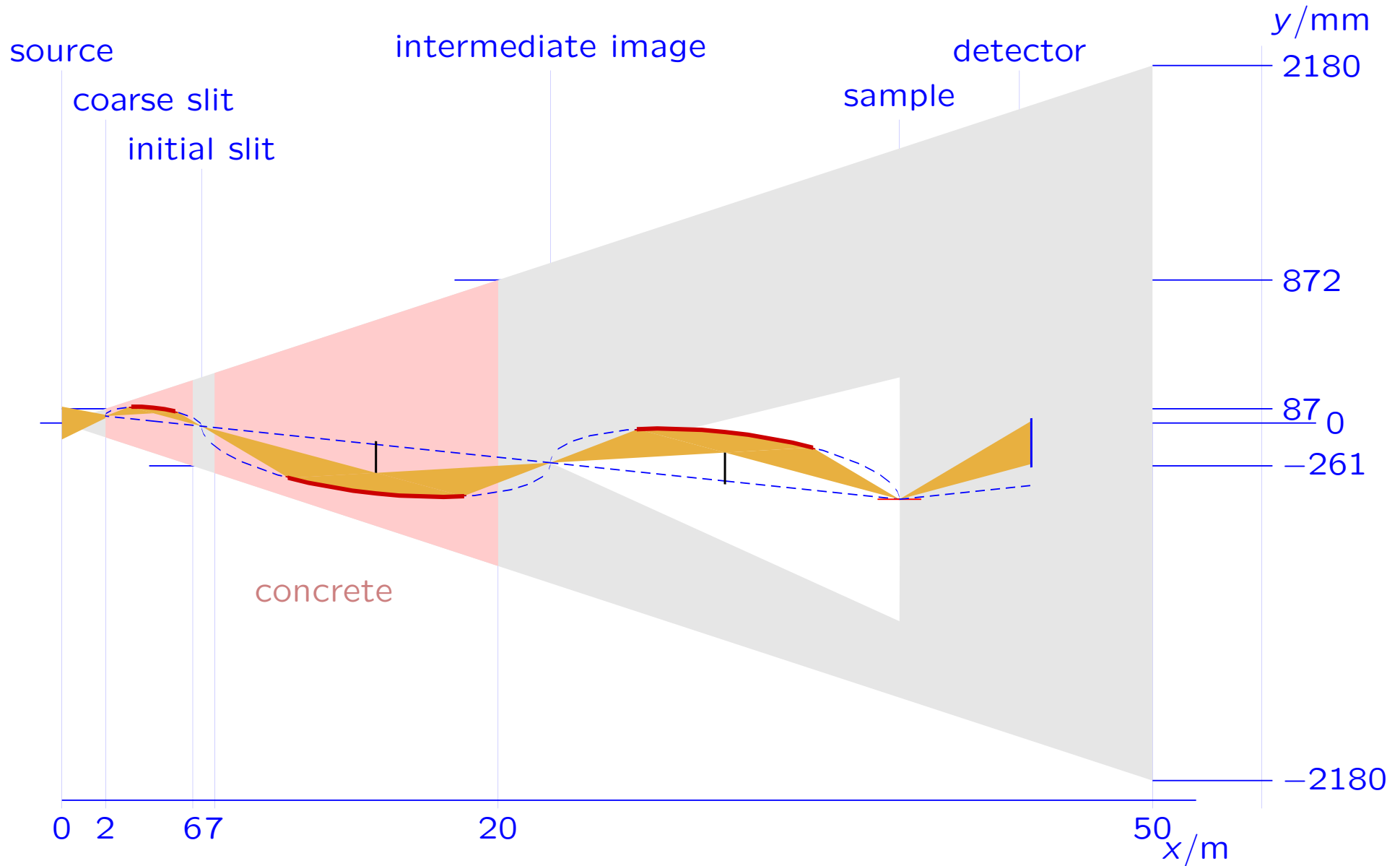
$\lambda \in [1.5, 12] \text{ \AA}$

polarized beam

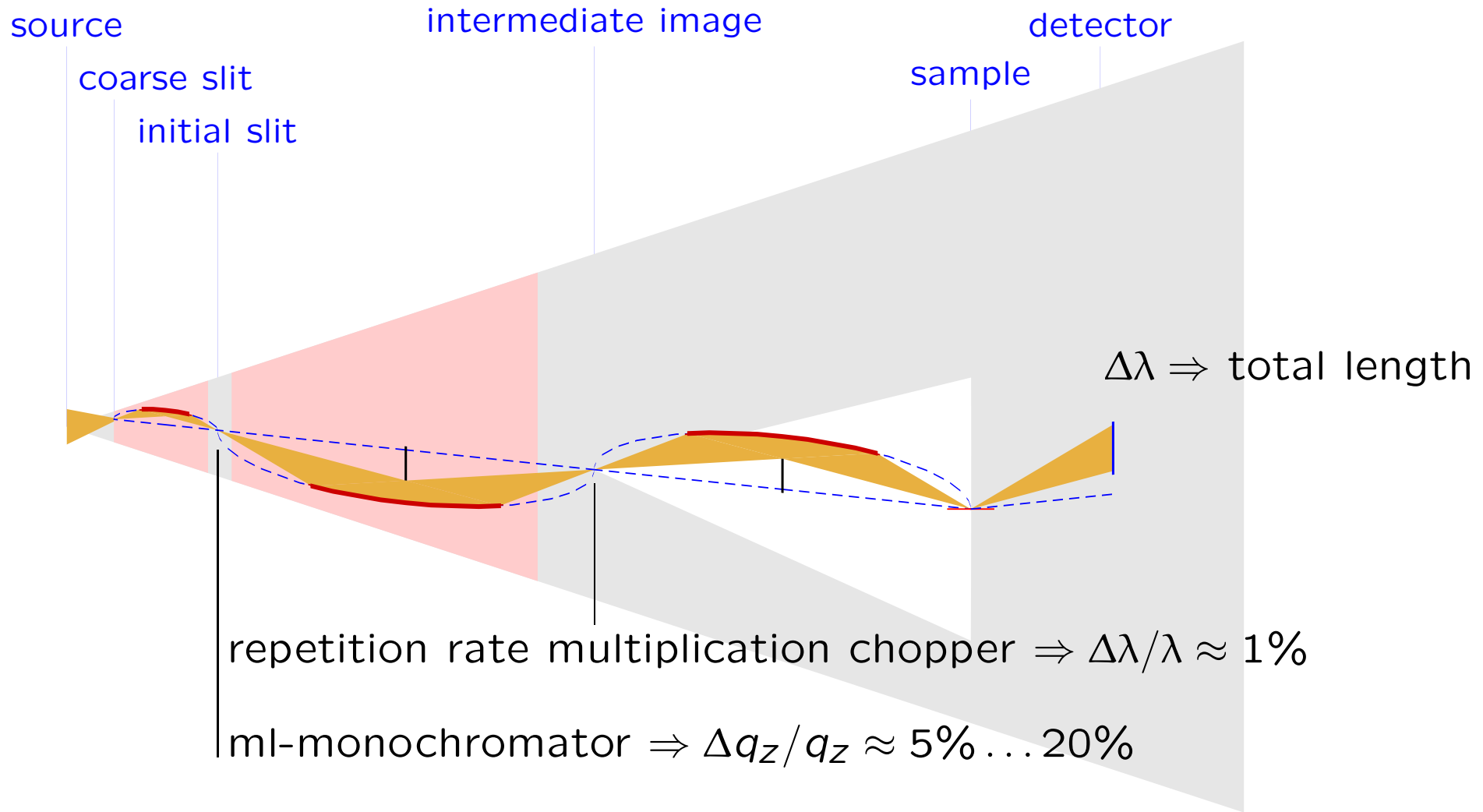
setup operational 8. 2012

realisation: concept for the ESS

schematic lay-out of the reflectometer for tiny samples



realisation: concept for the ESS

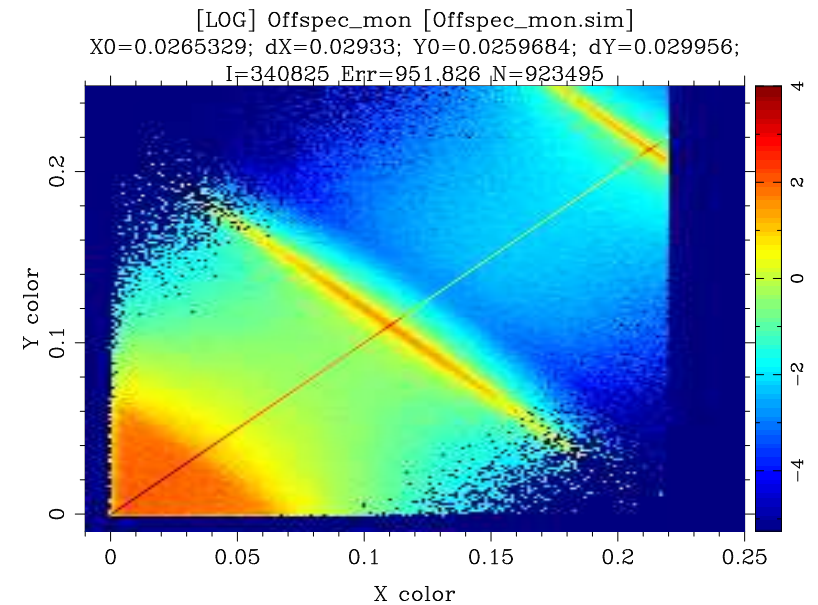


final remarks

critical points

- accuracy of guides
 - how to assemble the 0.5 m units without errors
- alignment of guides
- scattering at focal points
 - from diaphragms / choppers
 - off-specular form mirrors

first simulation with off-specular scattering with McStas
(K. Leffman, 12. 2011)



- influence of gravity
 - will be simulated within the next months

thanks to

Tobias Panzner McStas simulations, experiments, BOA
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Marité Cardenas experiments
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Hanna Wacklin discussions
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Peter Böni
Uwe Stuhr
Frederic Ott
Thomas Krist

Selene is a guide concept

which ...

- prevents direct line of sight
 - reduces radiation in the guide
 - allows for convenient beam manipulation
- reduces illumination of the sample environment
 - allows for a convergent beam set-up
⇒ flux gain > 10



URL: <http://people.web.psi.ch/stahn>

J. Stahn, *et al.* N.I.M. A **634**, S12 (2011)

J. Stahn, *et al.* Eur. Phys. J. Appl. Phys., doi:10.1051/epjap/2012110295