

Customizing Neutron Beams

Peter Böni

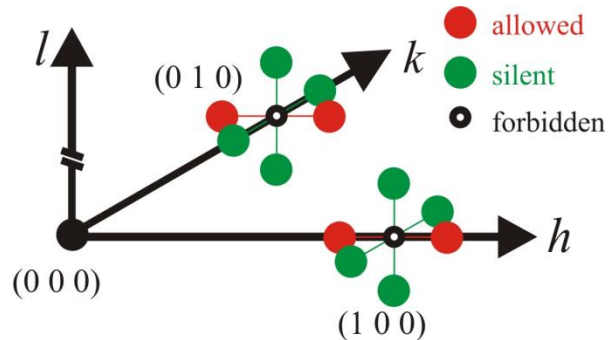
Physik-Department E21
Technische Universität München
D-85748 Garching

E-mail: Peter.boeni@frm2.tum.de

Web: www.sces.ph.tum.de

Strongly Correlated Electron Systems

Example: incommensurate Cr



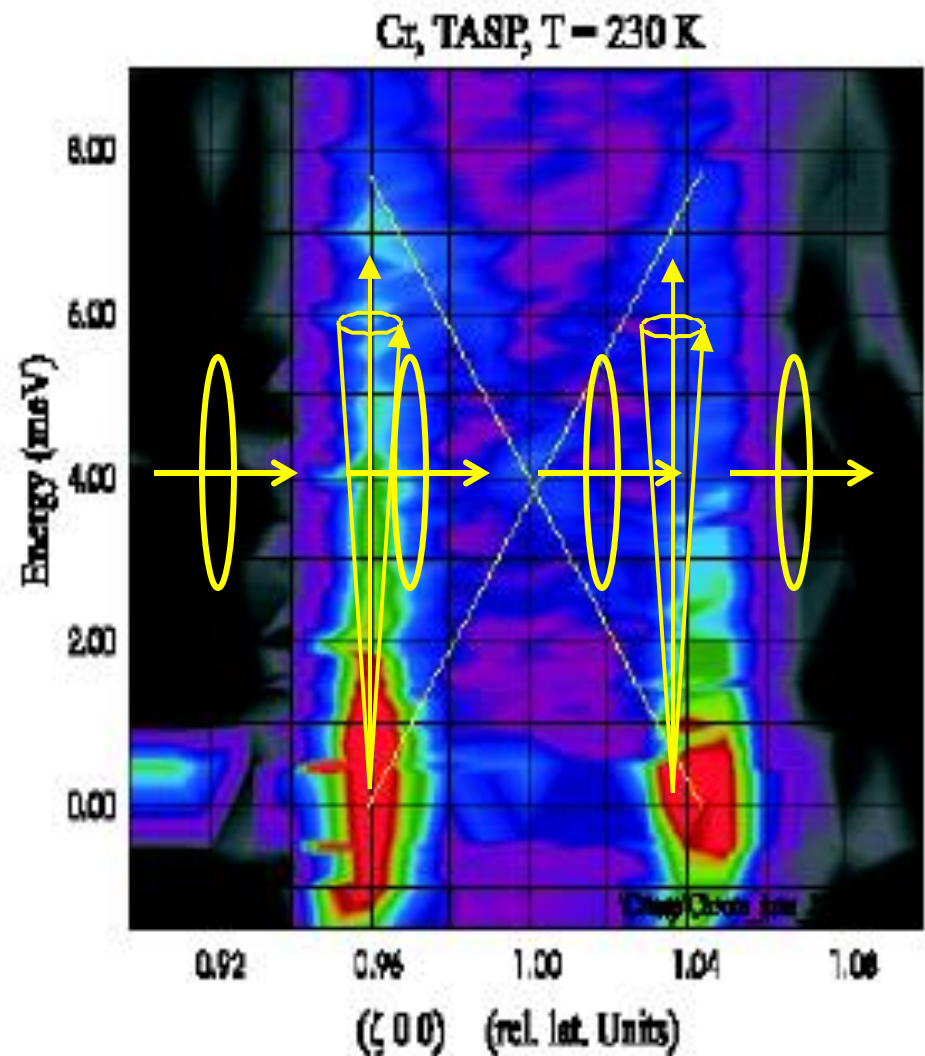
- extremely steep slope:

$$E_{SW} = cq \quad c = \frac{v_F}{\sqrt{3}}$$

- fine **Q**-resolution
- coarse **E**-resolution

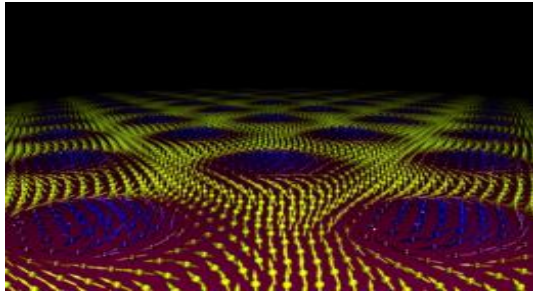
Further examples:

- high T_c superconductors
- strongly correlated electron systems

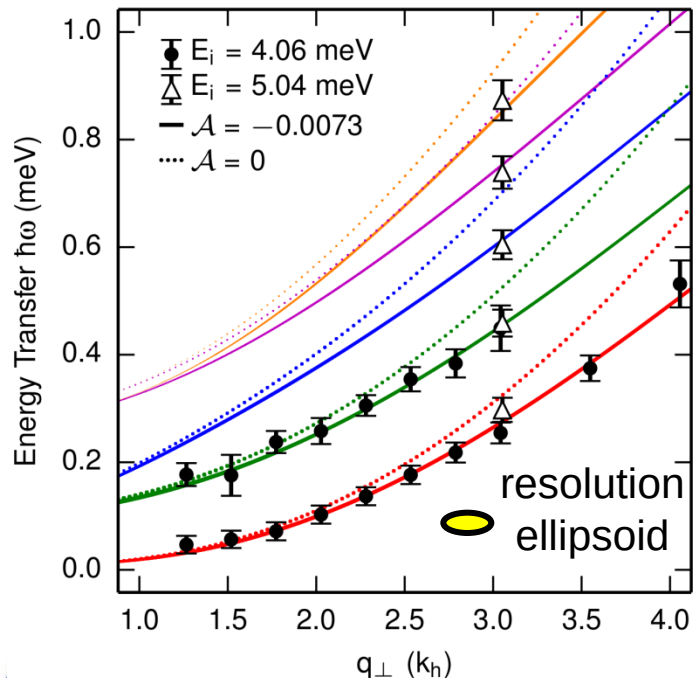


Smaller Samples and High Resolution: QPTs

Skyrmions in MnSi

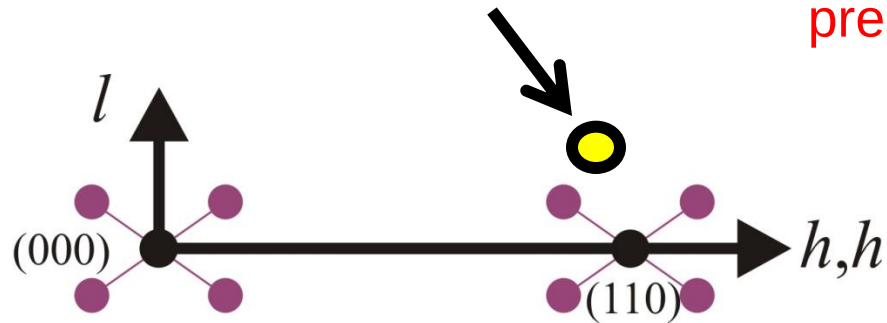
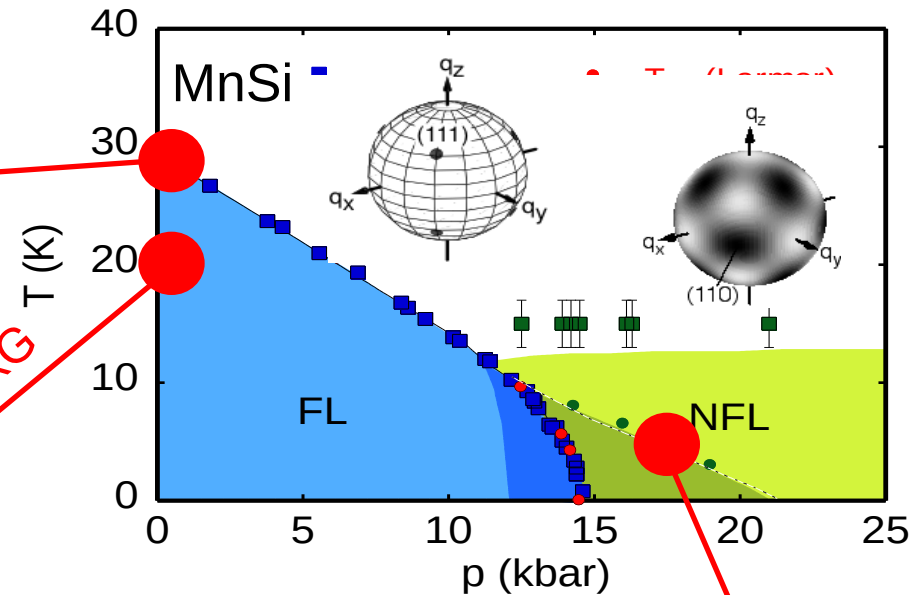


S. Mühlbauer et al., Science **323** (2009) 915



$B = 1.8$ kG

$B = 1$ kG

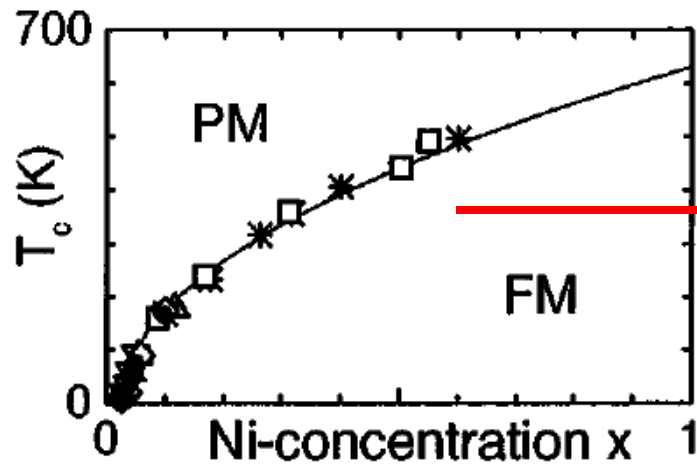


Excellent Q - and E -resolution required

QPT Using Doping $\leftrightarrow$ Homogeneity of Samples

$\text{Pd}_{1-x}\text{Ni}_x$: control parameter: x

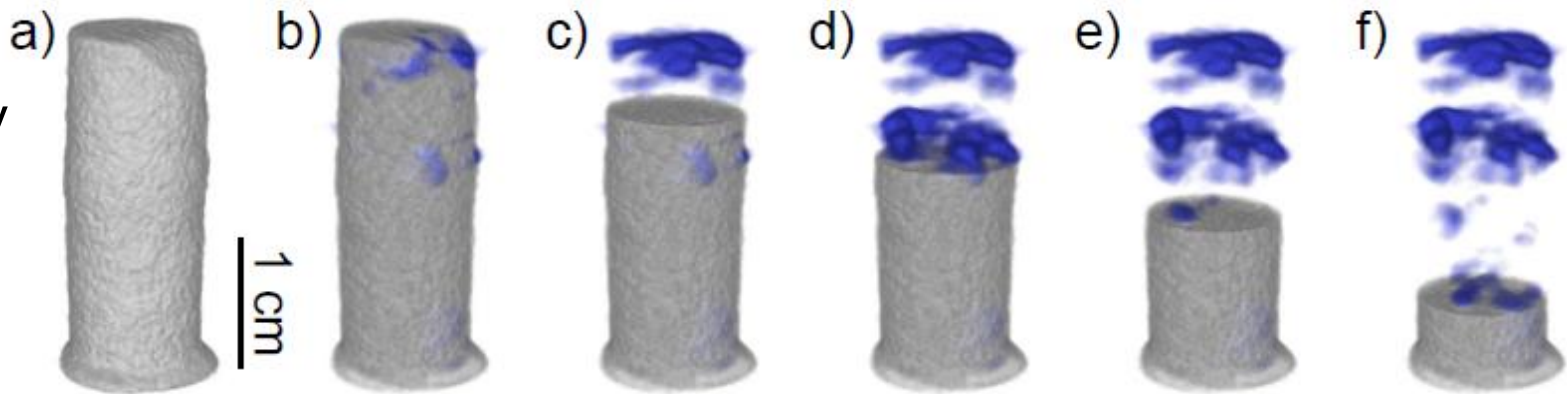
M. Nicklas et al., Phys. Rev. Lett. **82**, 4268 (1999)



single crystal:



tomography with
polarized
neutrons:

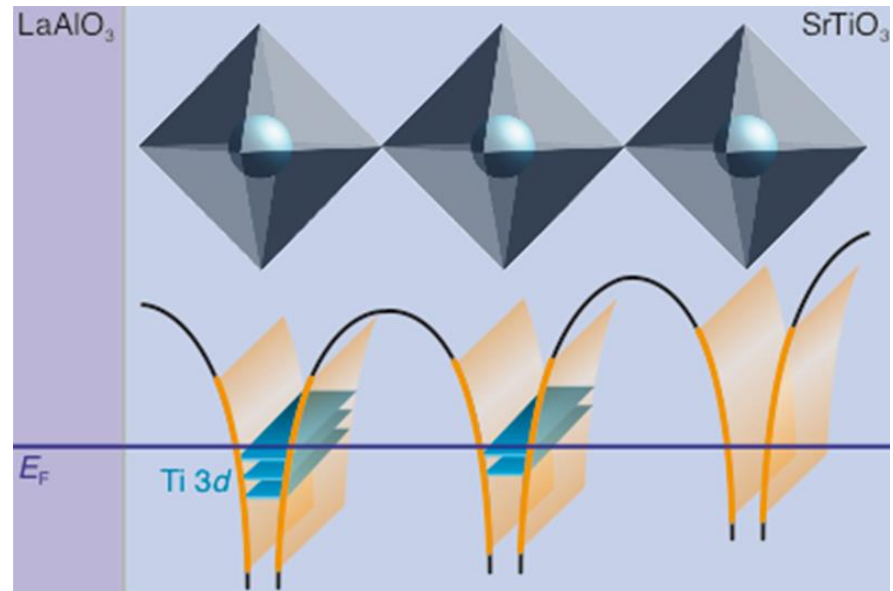
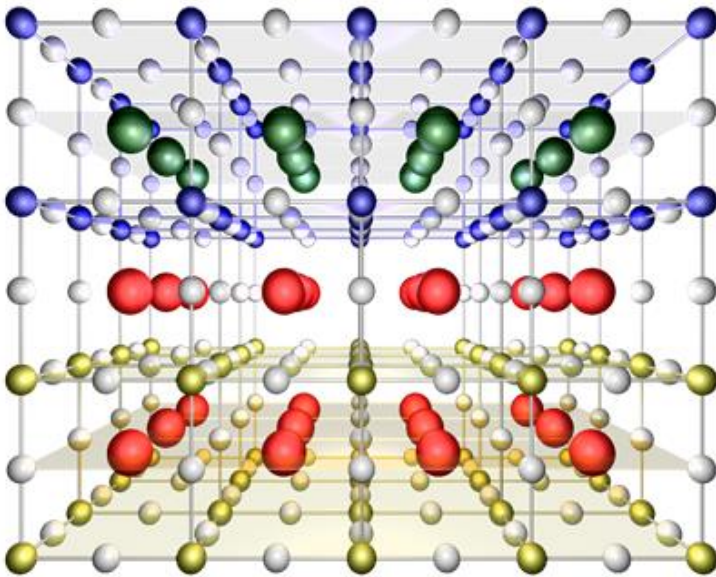


Apply position dependent scattering techniques

Heterostructures of Functional Oxides

$\text{SrTiO}_3/\text{LaAlO}_3$:

- control parameter: number of layers SrTiO_3 on LaAlO_3



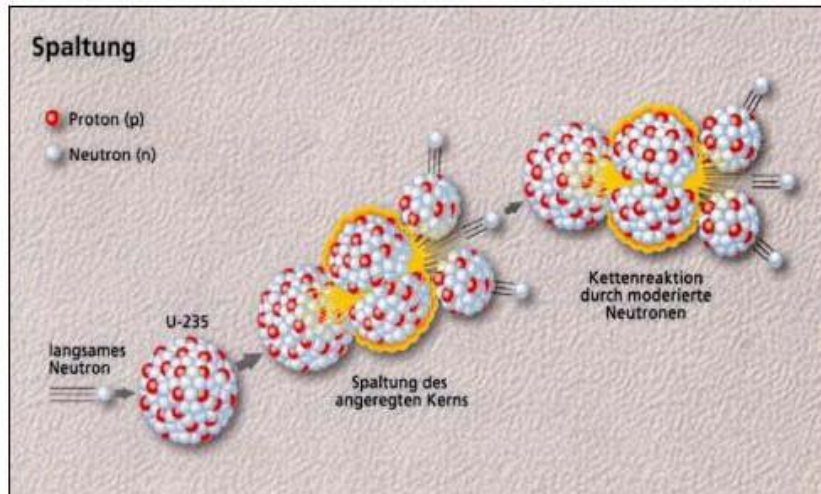
2-D electron liquid at the LaAlO_3 - SrTiO_3 interface: ferrom. / supercond.

monolayer samples → adaption of reflectometry for *in-situ* studies

Content

- Introduction
- Supermirrors
- Transport
- Focusing Optics
- Montel Mirrors
- Beam Extraction
- Summary

Production of Neutrons



fission

FRM-II, München

spallation

SINQ, Paul Scherrer Institut

→ ESS in Lund, Sweden

Some Pictures of Neutron Sources

ESS, Sweden



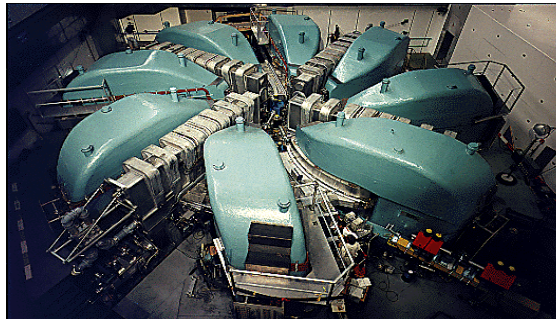
Chalk River, Canada



FRM II, Germany



SINQ, Switzerland



ILL, France



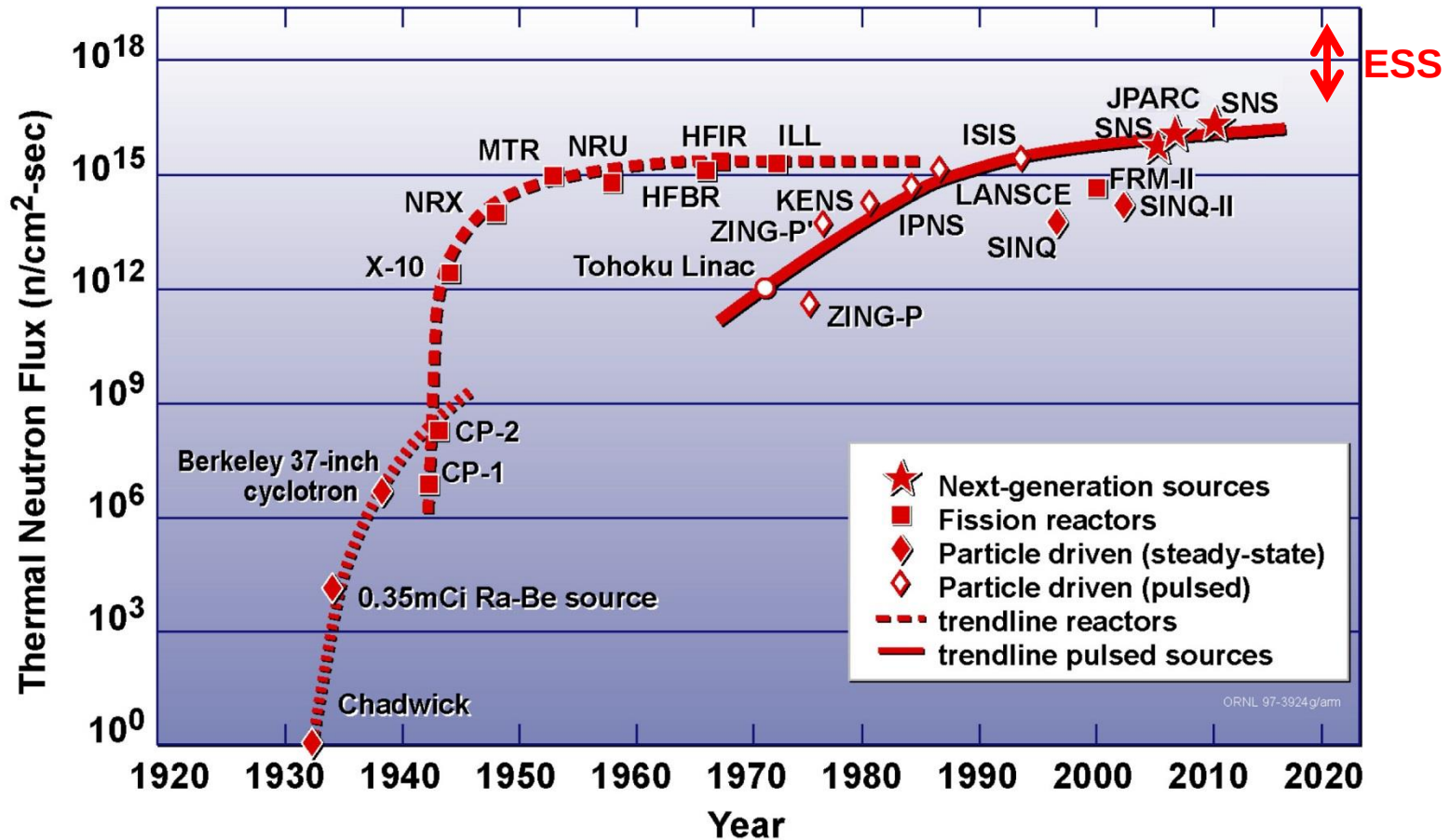
ISIS TS-2, UK



SNS, USA



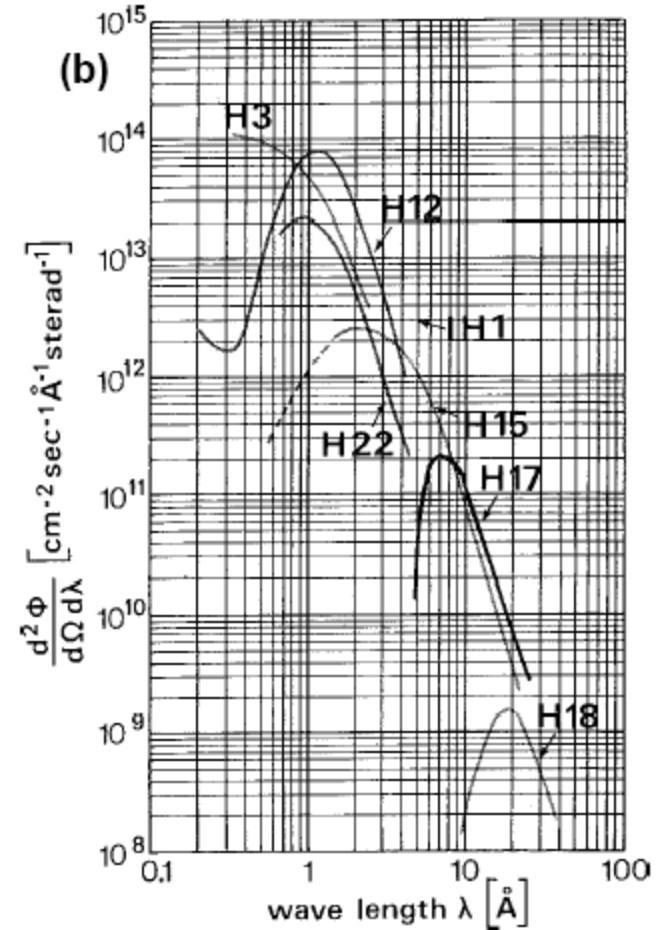
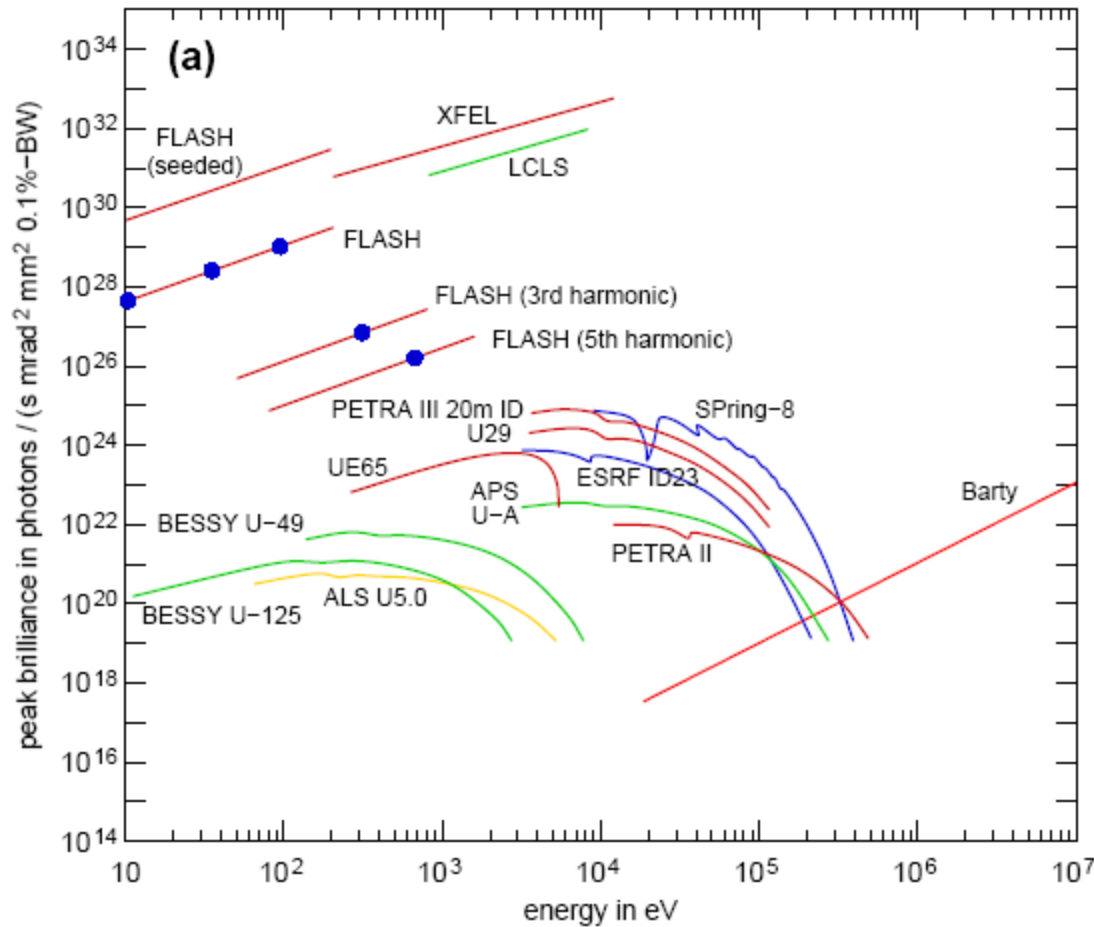
Flux of Neutron Sources



(Updated from *Neutron Scattering*, K. Skold and D. L. Price: eds., Academic Press, 1986)

Brilliance of X-ray and Neutron Beams

$$\Psi = \frac{d^2\phi}{d\Omega d\lambda} = \frac{1}{\text{cm}^2 \text{ s BW sterad}}$$



Difficult to compare for non-expert.

Brilliance of X-ray and Neutron Beams: Units!

$$\Psi = \frac{d^2\phi}{d\Omega d\lambda} = \frac{\text{neutrons}}{\text{cm}^2 \text{ s } \text{\AA} \text{ sterad}}$$

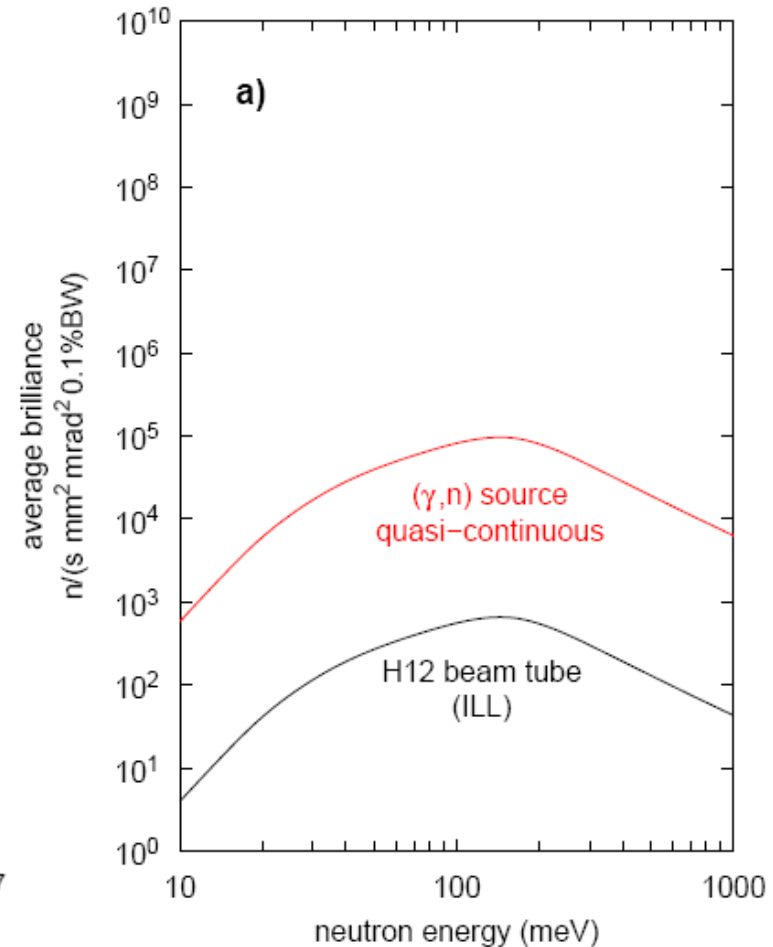
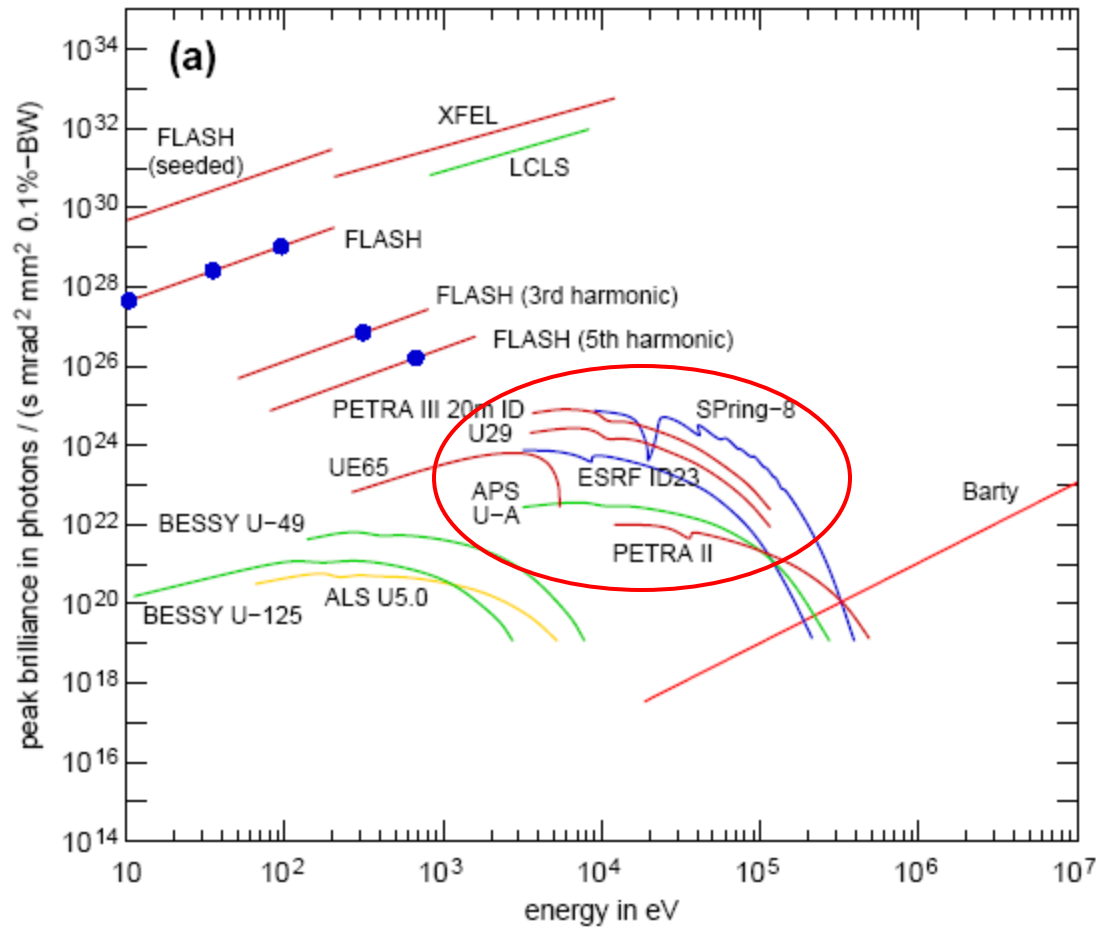
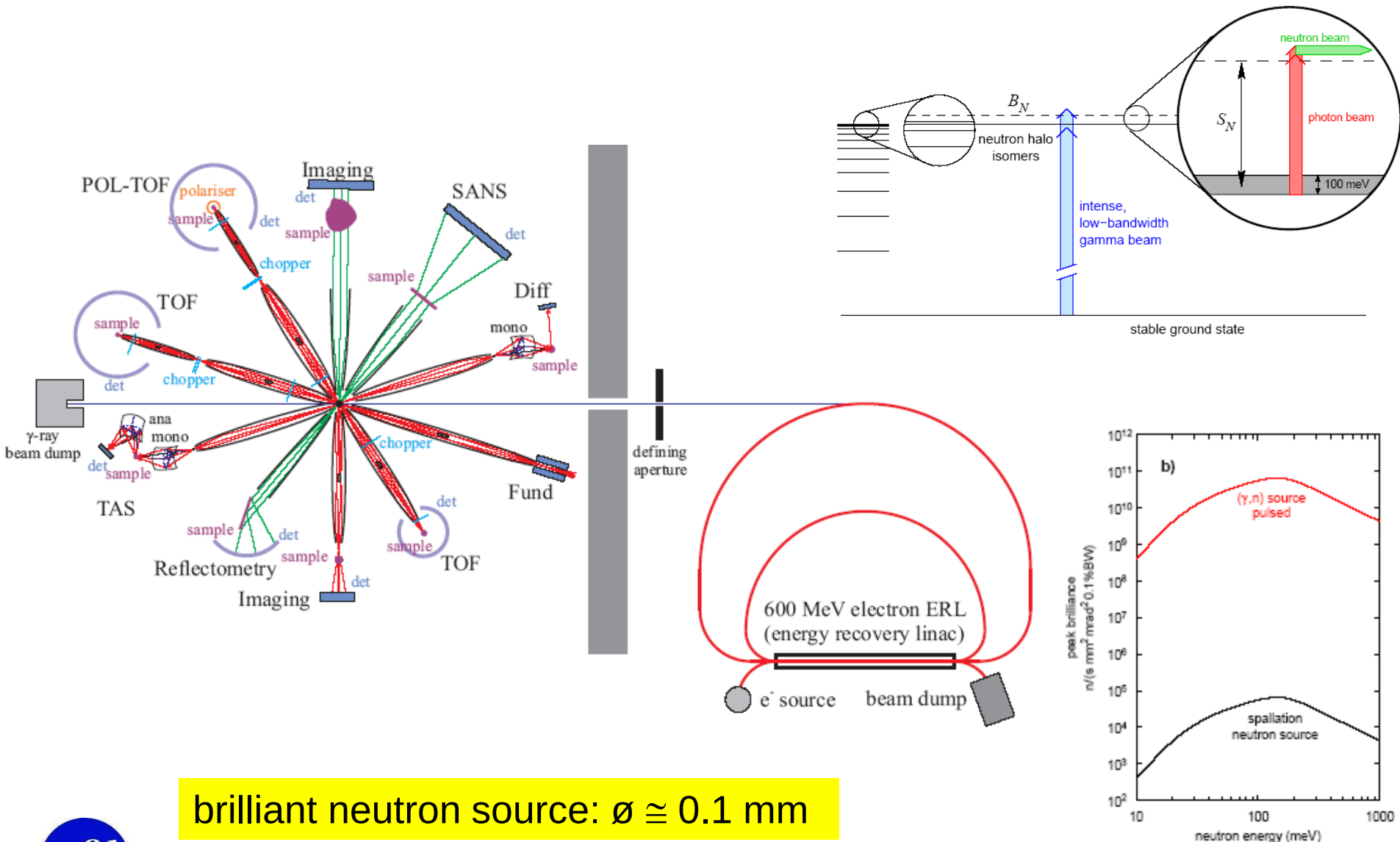


Photo-Neutrons from Halo Nuclei?



Performance of a Source

intensity:

- counts $\approx$ photons, neutrons, ...
- detection may not be 100% efficient

$$I = \frac{\text{counts}}{s}$$

flux:

$$\phi = \frac{1}{\text{cm}^2 \text{ s}}$$

brilliance:

- Ω : solid angle (sterad)
- λ : wavelength (Å)

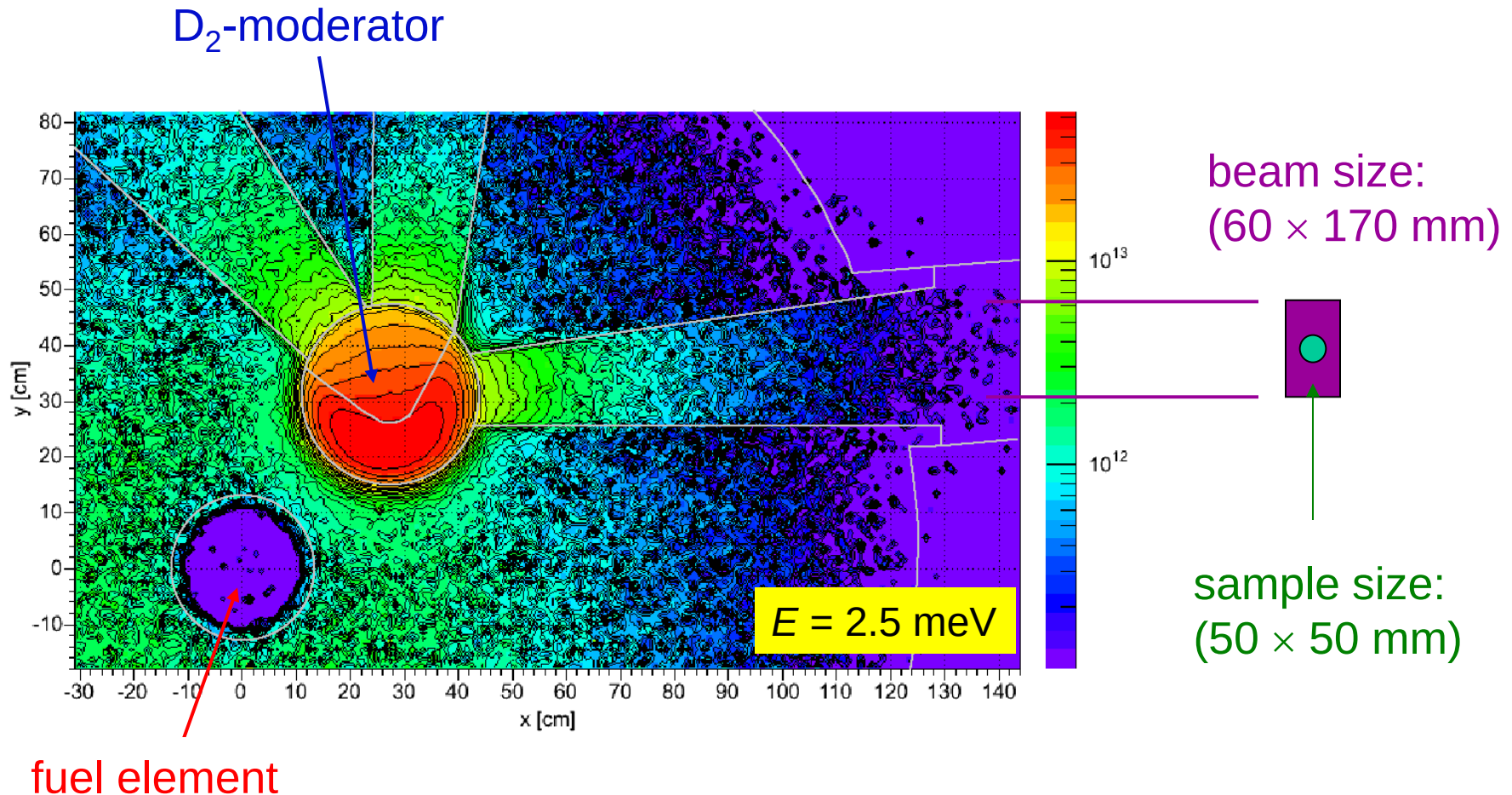
$$\Psi = \frac{d^2 \phi}{d\lambda d\Omega} = \frac{1}{\text{cm}^2 \text{ s } \text{\AA} \text{ sterad}}$$

The more the better?

Optimization Using Monte-Carlo Simulations (MCNPX)

FRM-II, Garching:

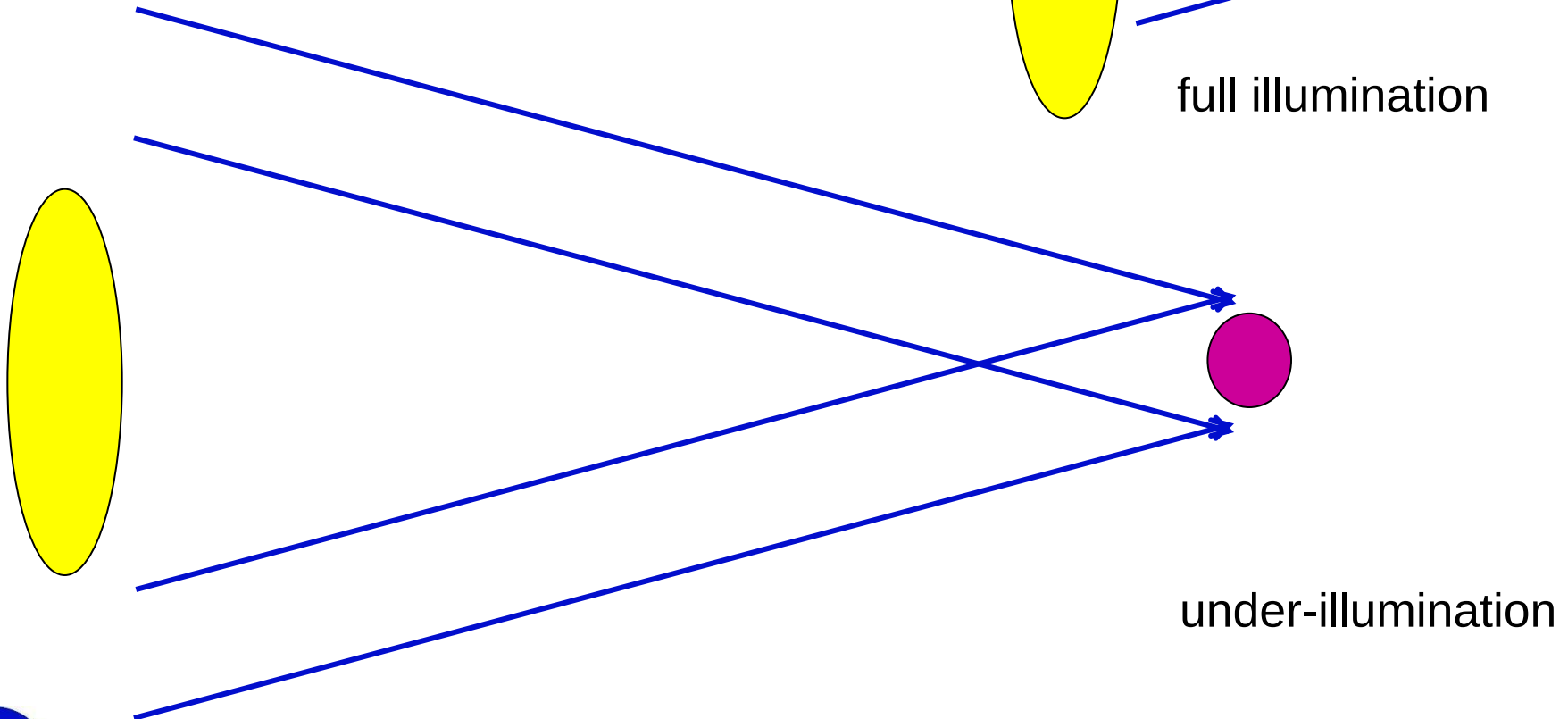
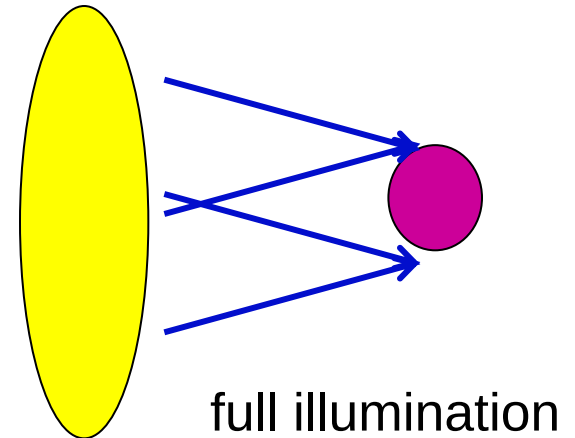
20'000 km/s $\rightarrow$ 2 km/s $\rightarrow$ 200 m/s



Illumination of a Sample

Reading a newspaper:

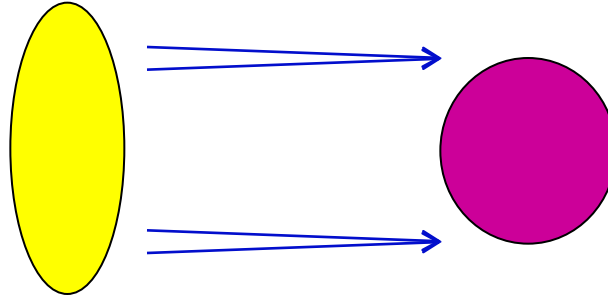
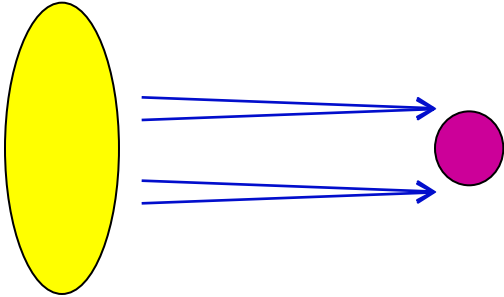
- go close to the light
- choose a bright light



Intensity (neutrons/s) Is Proportional to ...

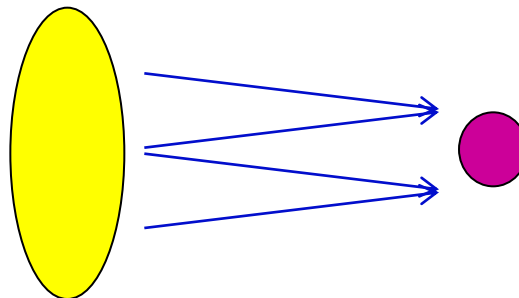
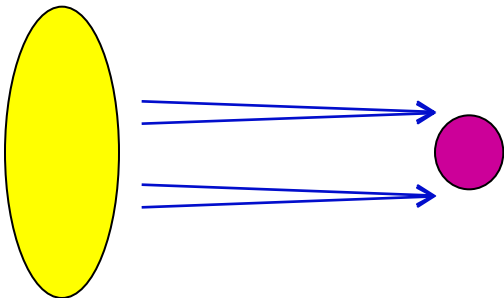
- sample size

(assumption: large source – full illumination)



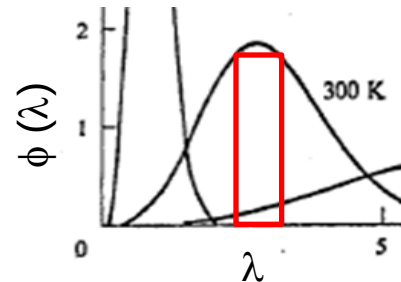
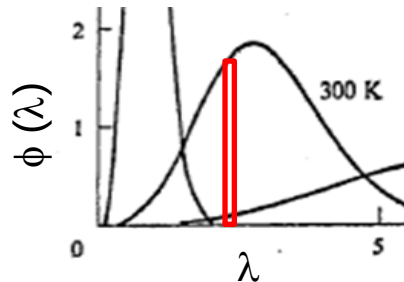
$A \text{ (cm}^2\text{)}$

- solid angle



$\Omega \text{ (sterad)}$

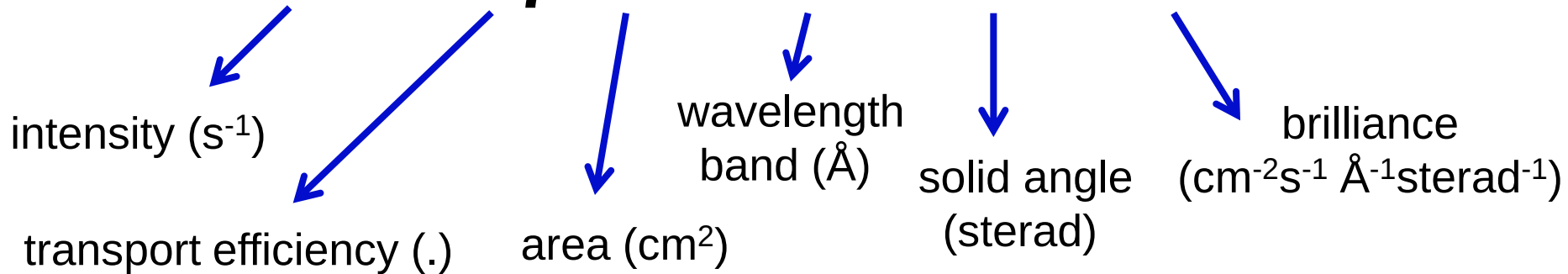
- band width



$\Delta\lambda \text{ (\AA}^{-1}\text{)}$

What is the Ultimate Intensity at the Sample?

$$I = \eta \cdot A \cdot \Delta\lambda \cdot \Omega \cdot \Psi$$



example: (Yellow Book of the ILL, p. 8, Fig. 4 (1986))

- port H12 @ ILL: $\Psi = 8 \cdot 10^{13} \text{ cm}^{-2}\text{s}^{-1} \text{\AA}^{-1}\text{sterad}^{-1}$ ($\lambda = 1.2 \text{ \AA}$)
- typical sample: $\eta = 0.5$, $A = 1 \text{ mm}^2$, $\Delta\lambda = 1\%$, divergence: $1^\circ/4^\circ$

→ Maximum neutron intensity at sample: $I = 5 \cdot 10^6 \text{ s}^{-1}$

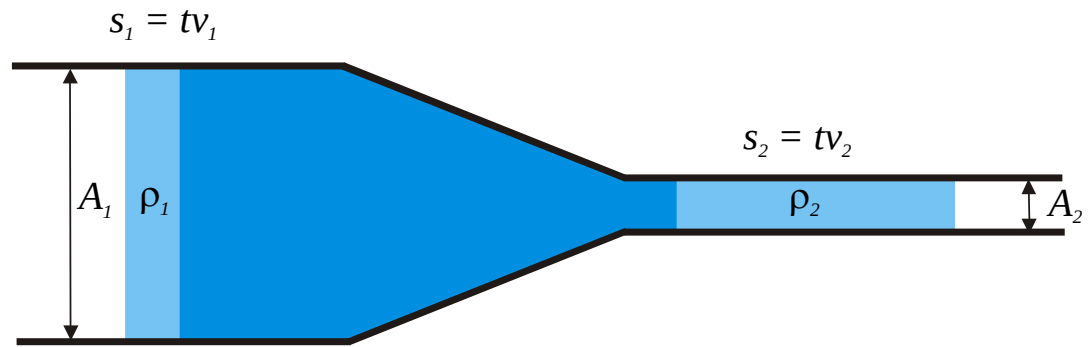
- experiment feasible?
 - intensity not achieved?
- technical limitations (SMs)
- refurbish beam line

Theorem of Liouville $\leftrightarrow$ Plumbing Heating

water pipes:

- fluid not compressible

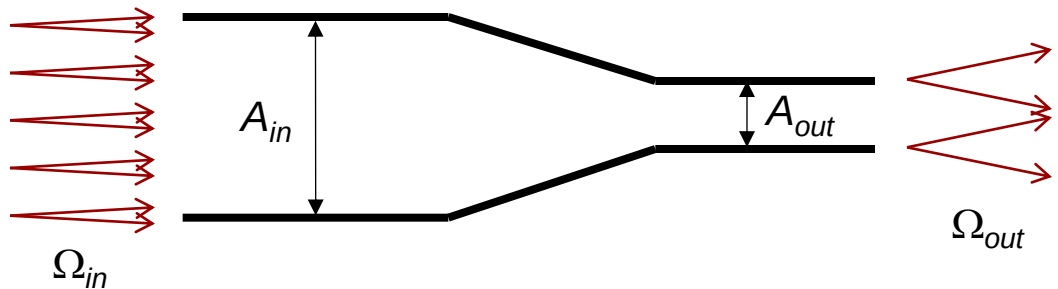
$$A_{in} v_{in} = A_{out} v_{out}$$



neutron transport:

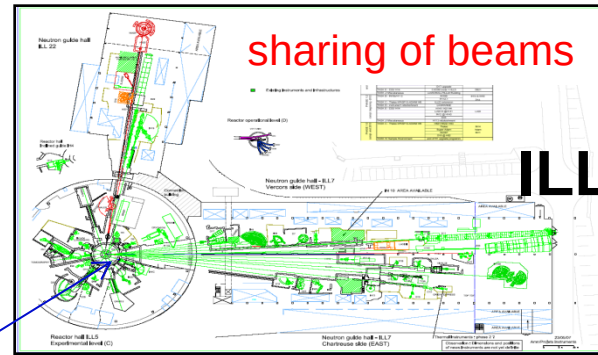
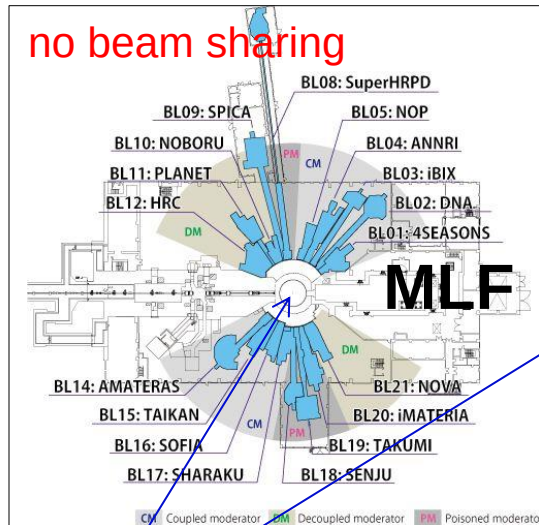
- Liouville: phase space density is constant in time
- neutrons do not change energy

$$A_{in} \Omega_{in} = A_{out} \Omega_{out}$$



We focus the beam by increasing the divergence!

Most Neutron Beams Are not Adapted to Sample



Liouville's theorem:
phase space density:

$$B = A \times \Omega = \text{const}$$

area $\times$ solid angle

used neutron beam:

- beam size: 1 cm $\times$ 1 cm
- divergence: 2° / 2°

$$\rightarrow B = 4 \text{ (cm}^0\text{)}^2$$

extracted neutron beam:

- beam size: 6 cm $\times$ 17 cm
- divergence: 1.5° / 1.5°

$$\rightarrow B = 230 \text{ (cm}^0\text{)}^2$$

balance: only ~2% of neutrons used!

- irradiation of materials $\rightarrow$ damage
- expensive shielding
- high background

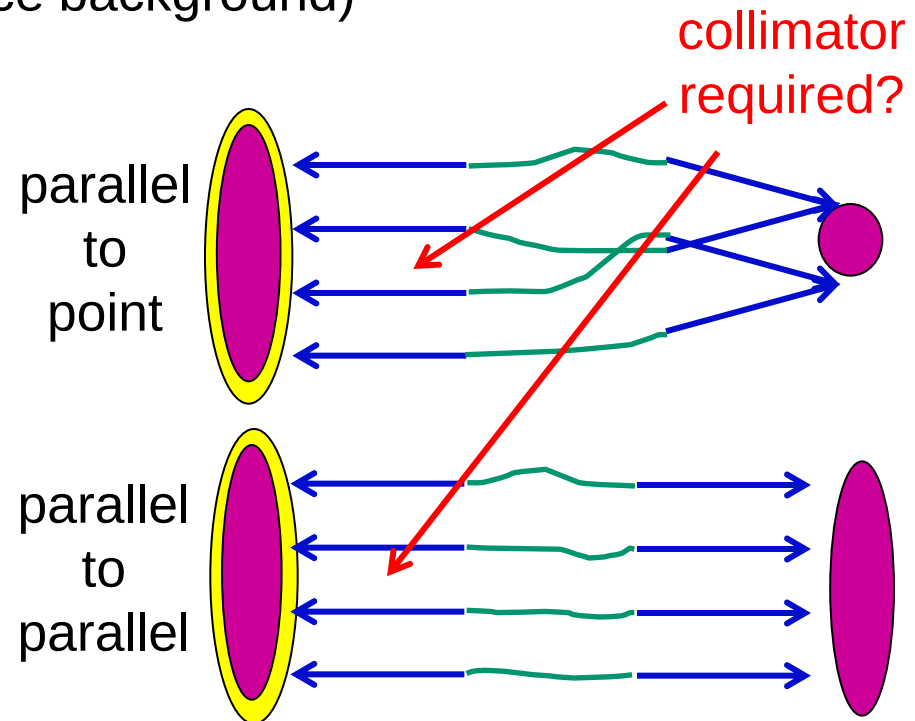
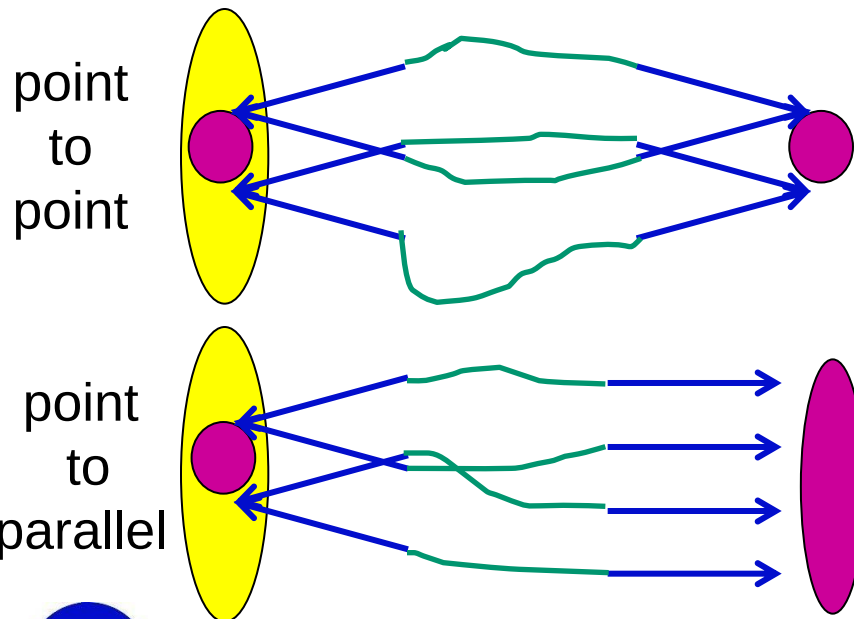
monochromatization: further reduction ($\sim 10^{-4}$)

Summary

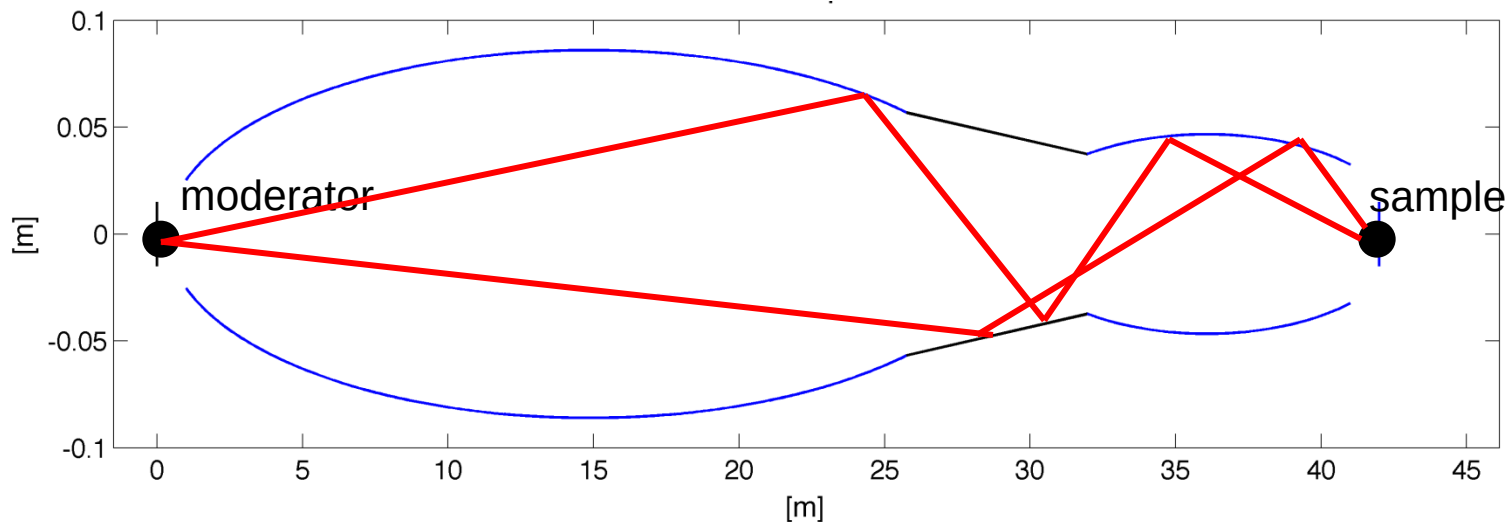
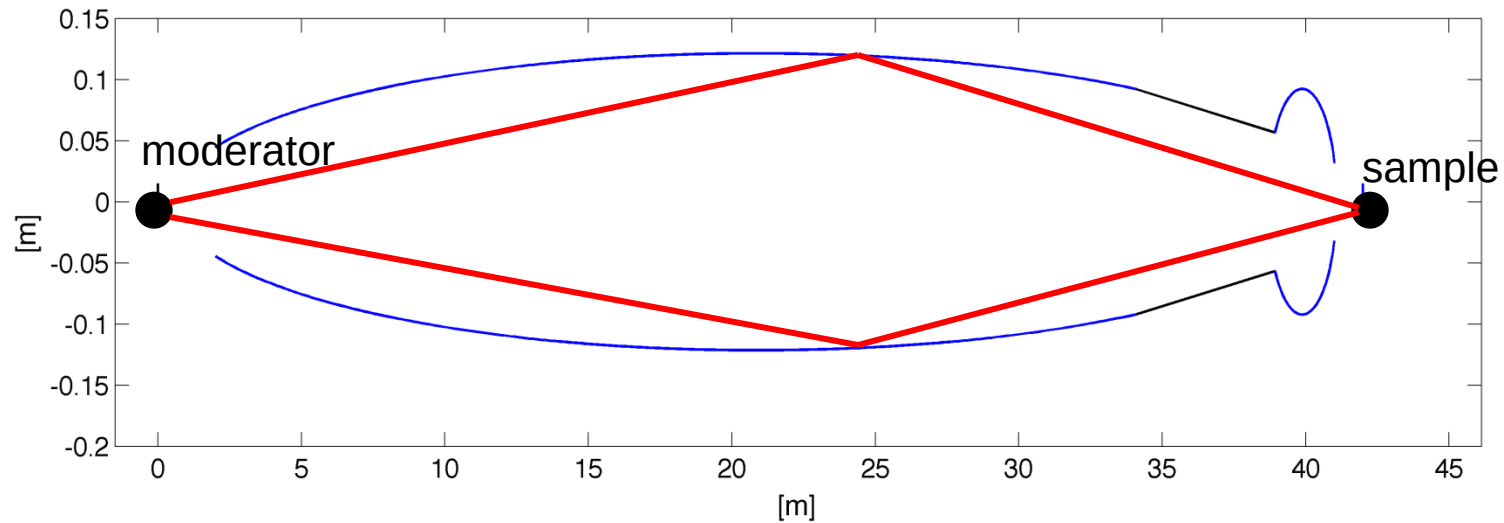
suggested procedure:

- define task of beam line:
 - sample size
 - divergence
 - band width, etc.
- calculate intensity at sample position ($\eta = 1$): experiment feasible?
- extract only useful neutrons (to reduce background)
- do not dilute phase space

$$I = A \cdot \Delta\lambda \cdot \Omega \cdot \Psi$$



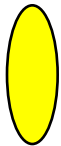
The Computer Does it for You



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Guide Neutrons $\leftrightarrow$ Compare Optical Fibers



moderator

neutron guide

beam line

Reflection from Surfaces 1

- interaction neutron – nuclei: $V(\mathbf{r}) = \sum_j b_j \delta(\mathbf{r}_j - \mathbf{r})$

- Schrödinger equation:

$$\frac{\hbar^2}{2m_n} \nabla^2 \psi + (E - V(\mathbf{r}))\psi = 0$$

- neutrons in vacuum:
(outside sample)

$$E_{\text{free}} = \frac{\hbar^2}{2m_n} k_i^2$$

- structure factor of sample:

$$F_{\tau} = \sum_j b_j e^{i\tau \cdot \mathbf{d}_n} e^{-W_n}$$

- potential in terms of F_{τ} :

$$V(\mathbf{r}) = \frac{\hbar^2}{2m_n} \frac{4\pi}{V} \sum_{\tau} F_{\tau} e^{-i\tau \cdot \mathbf{r}}$$

- forward scattering:

$$(\tau = 0) \quad V_0(\mathbf{r}) = \frac{\hbar^2}{2m_n} \frac{4\pi}{V} F_0 = \frac{\hbar^2}{2m_n} \frac{4\pi}{V} \sum_j b_j = \frac{\hbar^2}{2m_n} \frac{4\pi}{V} N \langle b \rangle = \frac{\hbar^2}{2m_n} 4\pi \rho \langle b \rangle$$

Complementarity between Neutron and Synchrotron X-Ray Scattering, Proceedings of the 6th Summer School on Neutron Scattering, edited by A. Furrer (World Scientific, Singapore, 1998), 305-327.

Reflection from Surfaces 2

Repetition:

- potential:
($\rho = N/V$: density)
($\langle b \rangle$: coherent scattering length)

$$V_0(\mathbf{r}) = \frac{\hbar^2}{2m_n} 4\pi\rho\langle b \rangle$$

- Schrödinger equation:

$$\frac{\hbar^2}{2m_n} \nabla^2 \psi + (E - V_0(\mathbf{r}))\psi = 0$$

$\swarrow \quad \downarrow \quad \searrow$
 $k_i^2 \quad -k^2 \quad 4\pi\rho\langle b \rangle$

- therefore:

- typically: $4\pi\rho\langle b \rangle < 10^{-4} k_i^2$

$$-k^2 + k_i^2 - 4\pi\rho\langle b \rangle = 0$$

$$k_i^2 - k^2 \cong 2k_i \updownarrow (k_i - k)$$

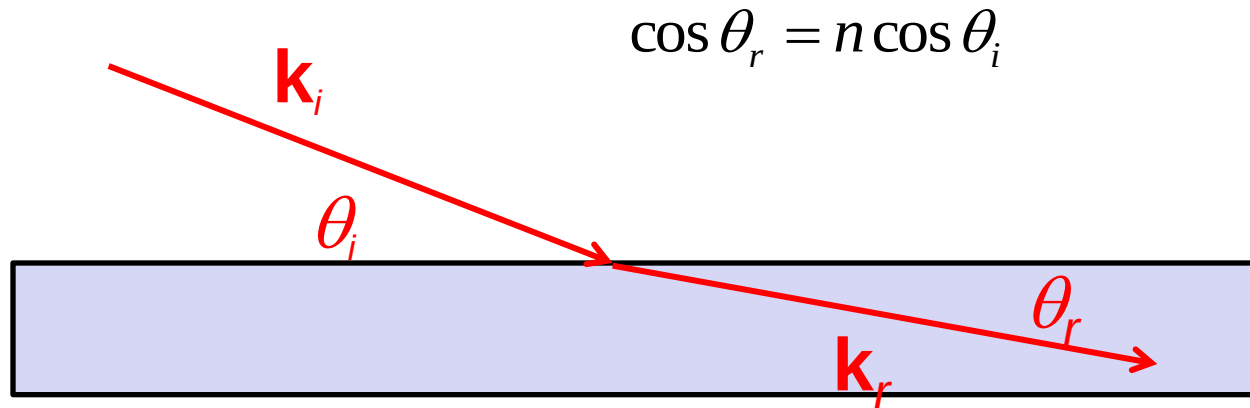
- index of refraction:

$$n = \frac{k}{k_i} = 1 - \frac{1}{2\pi} \rho\langle b \rangle \lambda^2$$

$n \propto \lambda^2$

Compare with Light Optics: Total Reflection

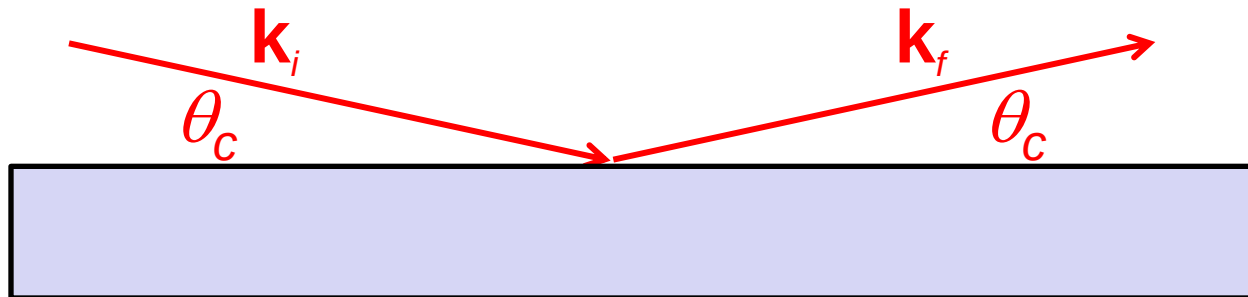
- Snell's law:



- total reflection:

$$\cos \theta_c = n$$

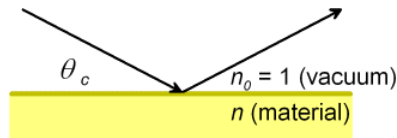
$$\theta_c^{Ni} (^{\circ}) = 0.1 \lambda (\text{\AA})$$



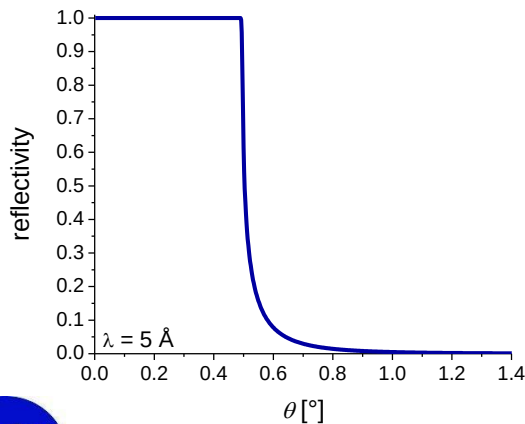
Extend Angle of Total Reflection: Supermirror

(Turchin 1976, Mezei 1976)

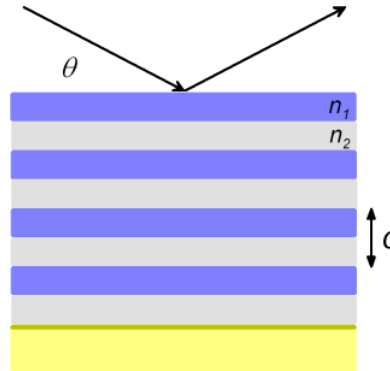
smooth surfaces



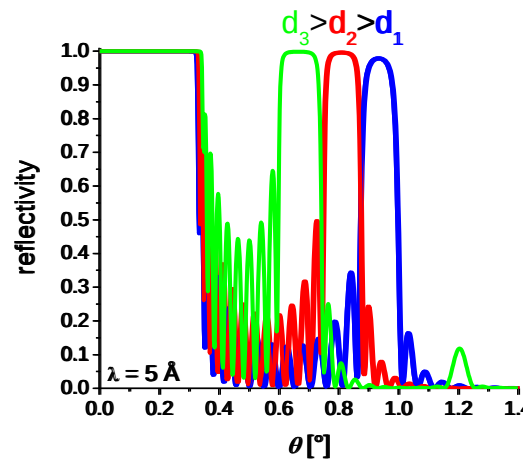
- useful for cold neutrons
($\lambda \cong 5 \text{ \AA}$)



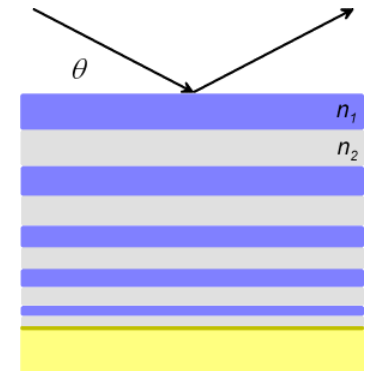
multilayer



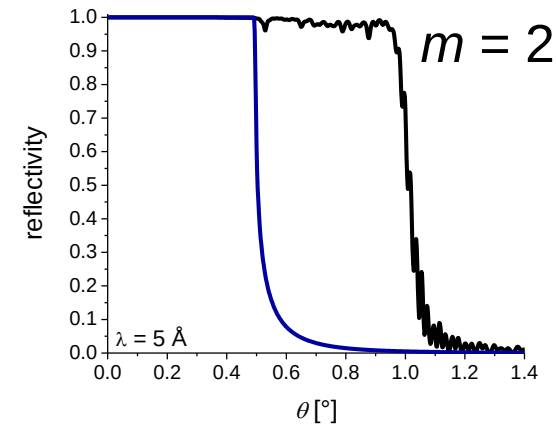
$$\lambda = 2d \sin \theta$$



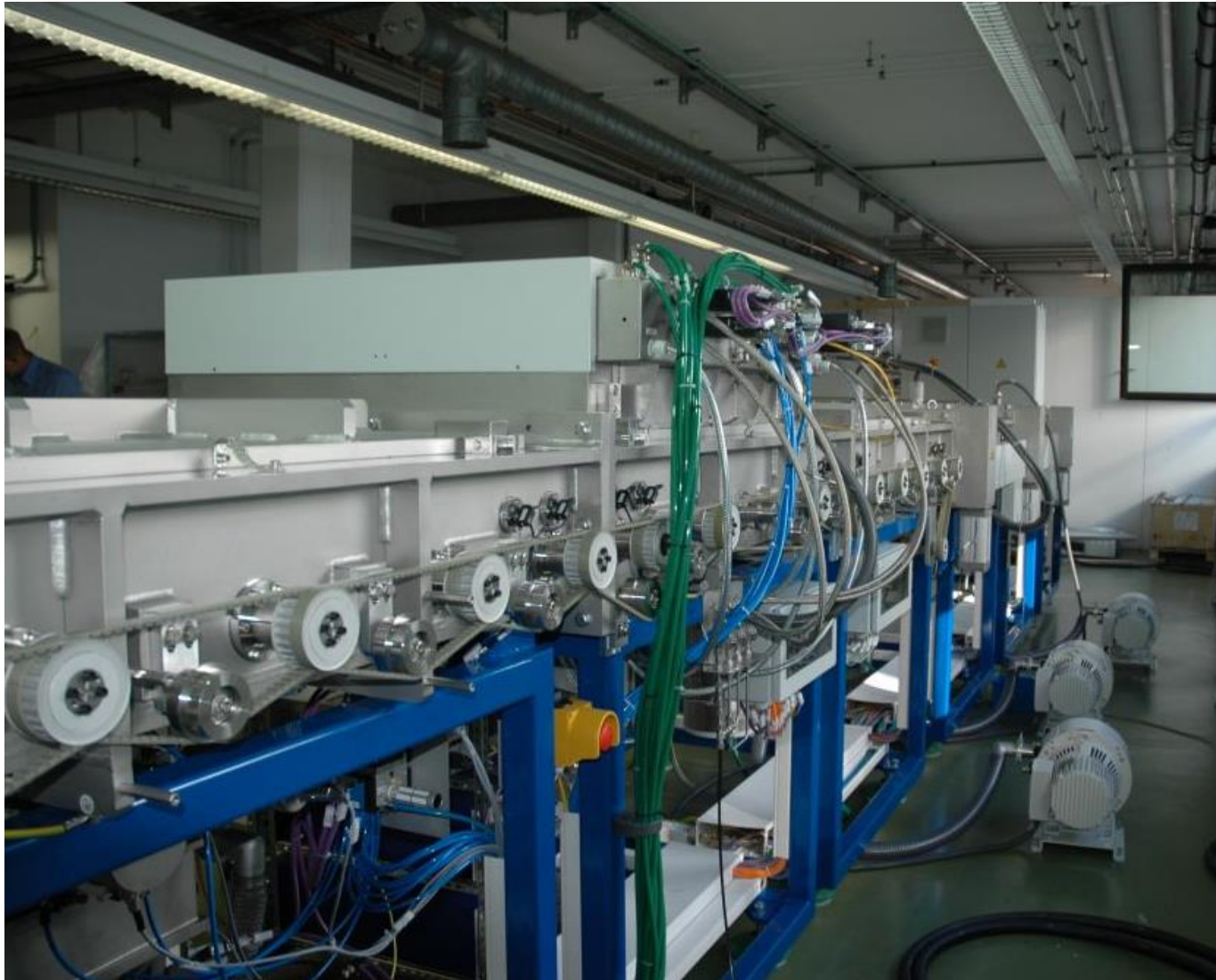
supermirror



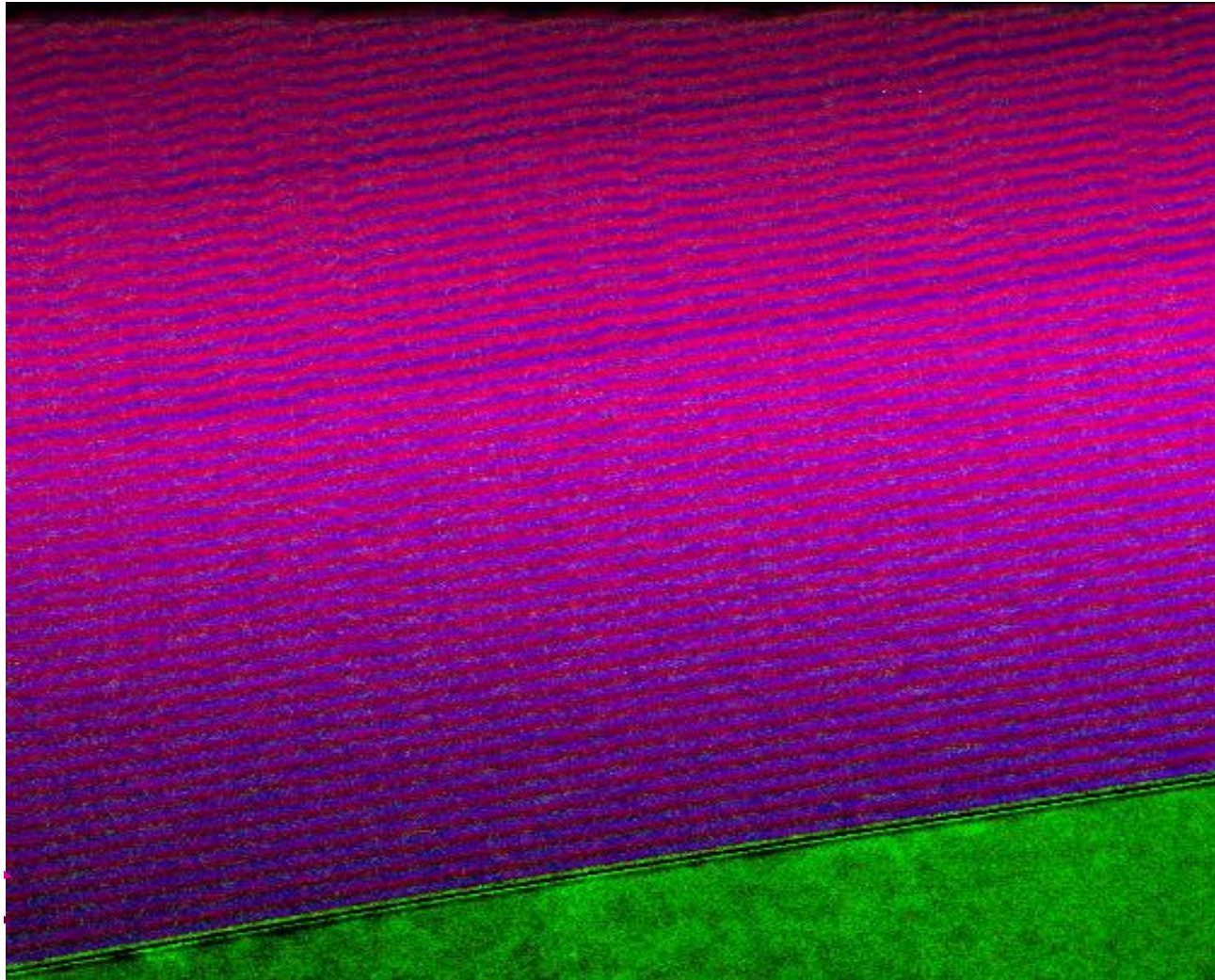
prevailing opinion:
- for cold neutrons only



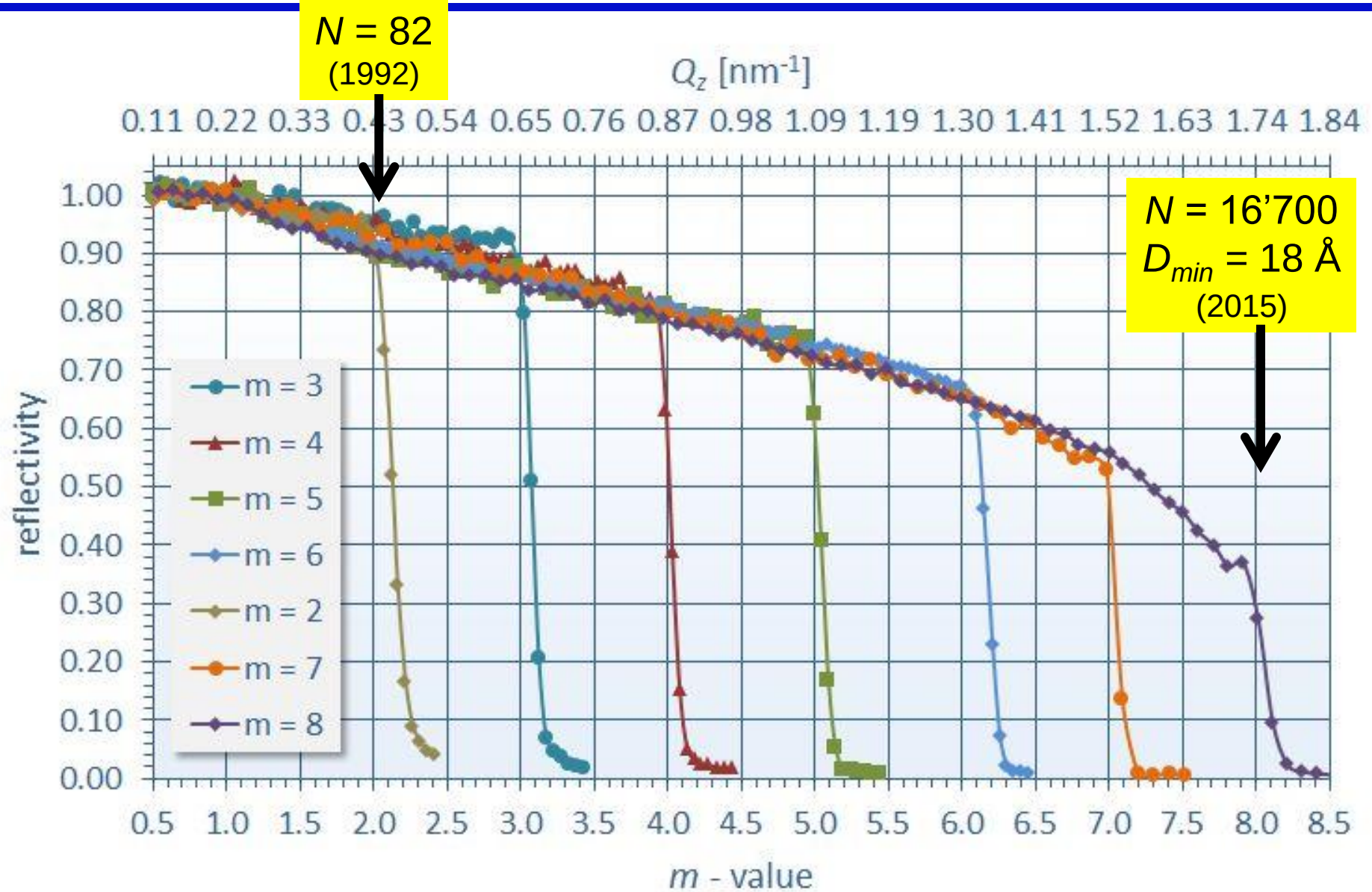
New Coating Processes $\rightarrow$ Larger θ_c



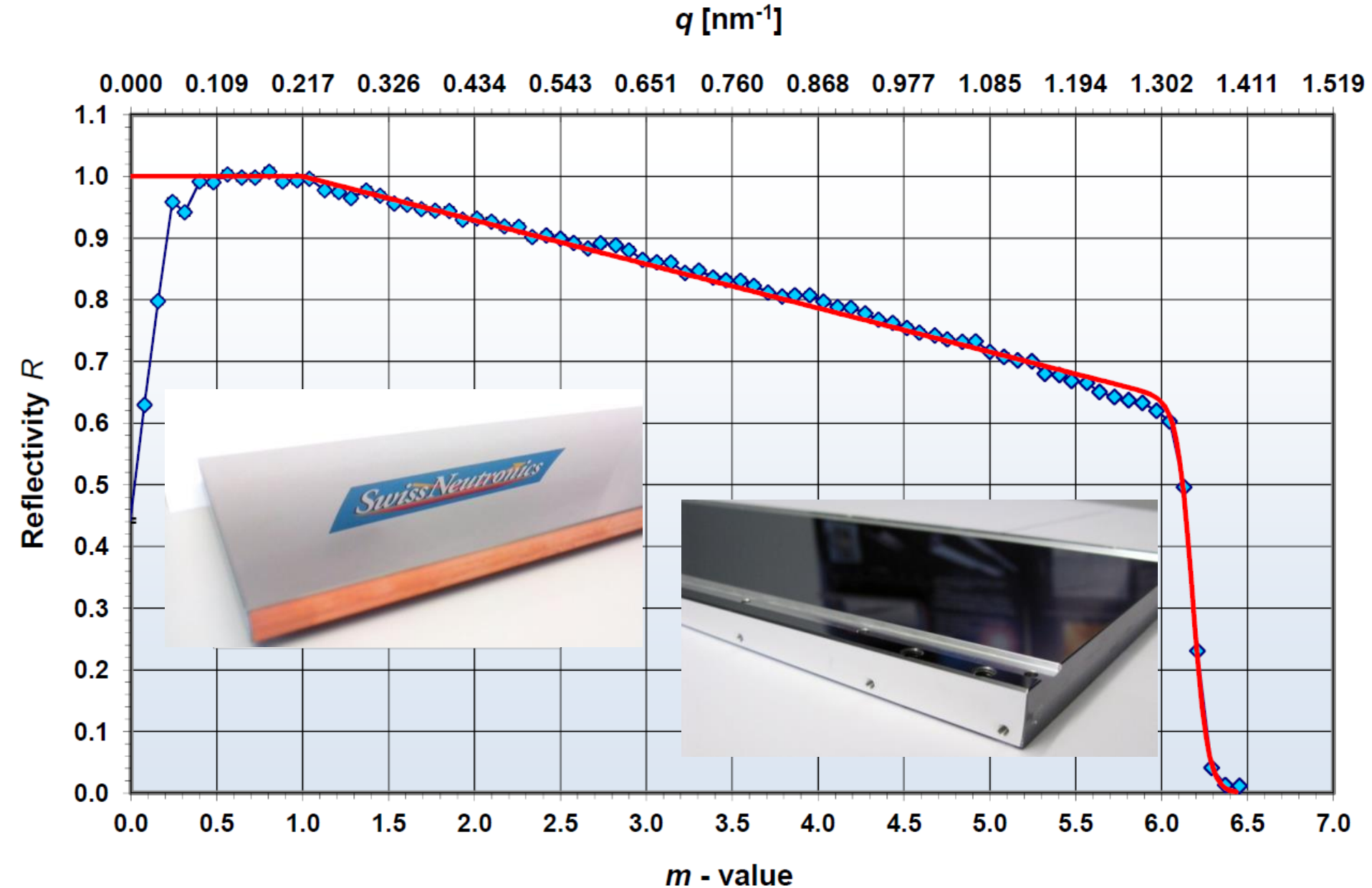
View by Transmission Electron Microscopy



Supermirror: State of the Art



Supermirror on Atomically Smooth Metal Substrates



Modern Supermirrors: large m , large R

large divergence available:

- extension of critical angles $\rightarrow$ large divergence α $1 \text{ \AA}$

thermal: $\alpha(1 \text{ \AA}) \cong 2 \cdot 0.1 \cdot 8 \cdot \lambda = 1.6^0$ $0.5 \text{ \AA}$

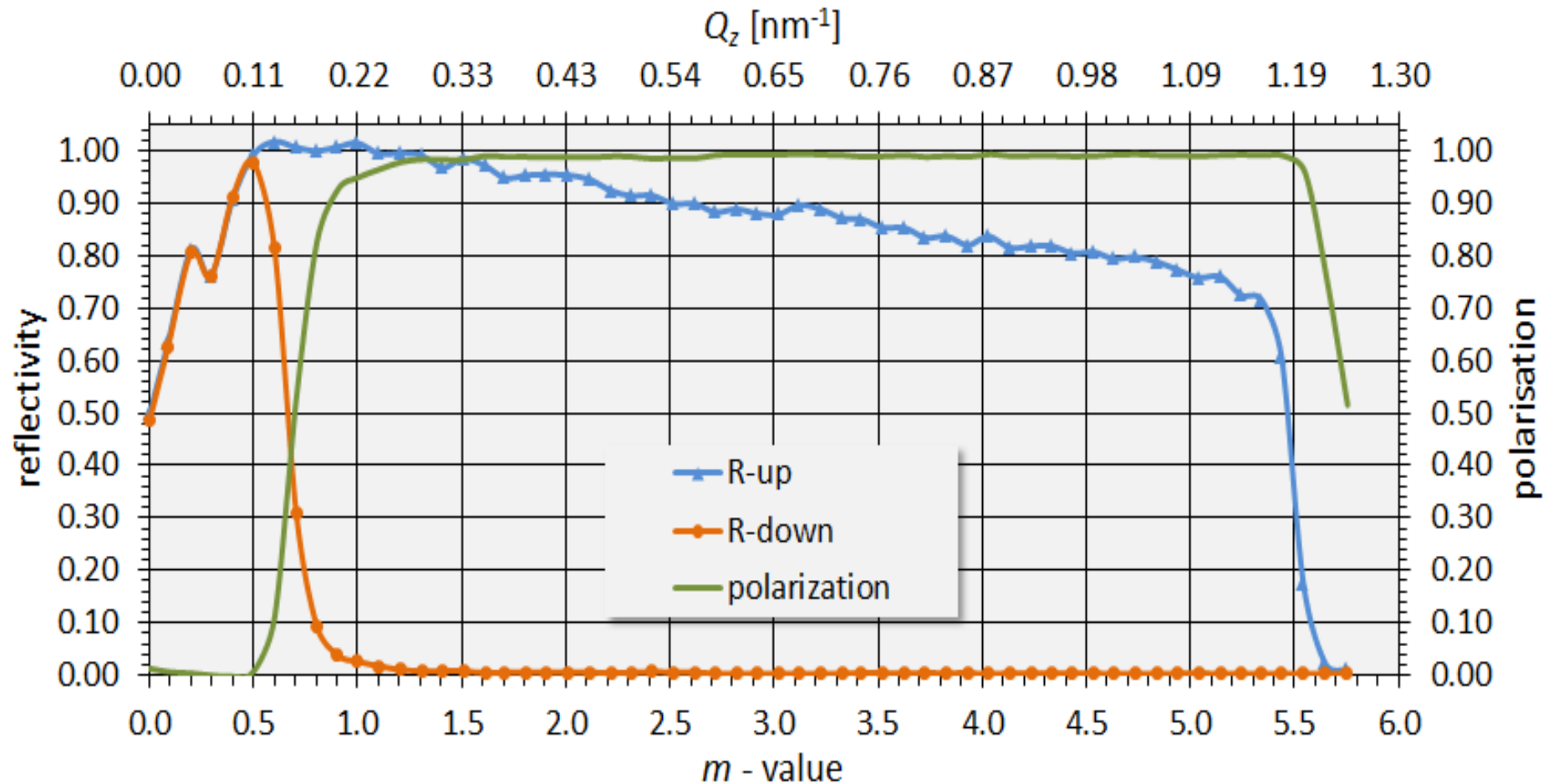
epithermal: $\alpha(0.5 \text{ \AA}) \cong 2 \cdot 0.1 \cdot 8 \cdot \lambda = 0.8^0$

- applications for hot (and epithermal?) neutrons possible
 $\rightarrow$ required for spallation sources!

efficient polarizers: Fe/Si

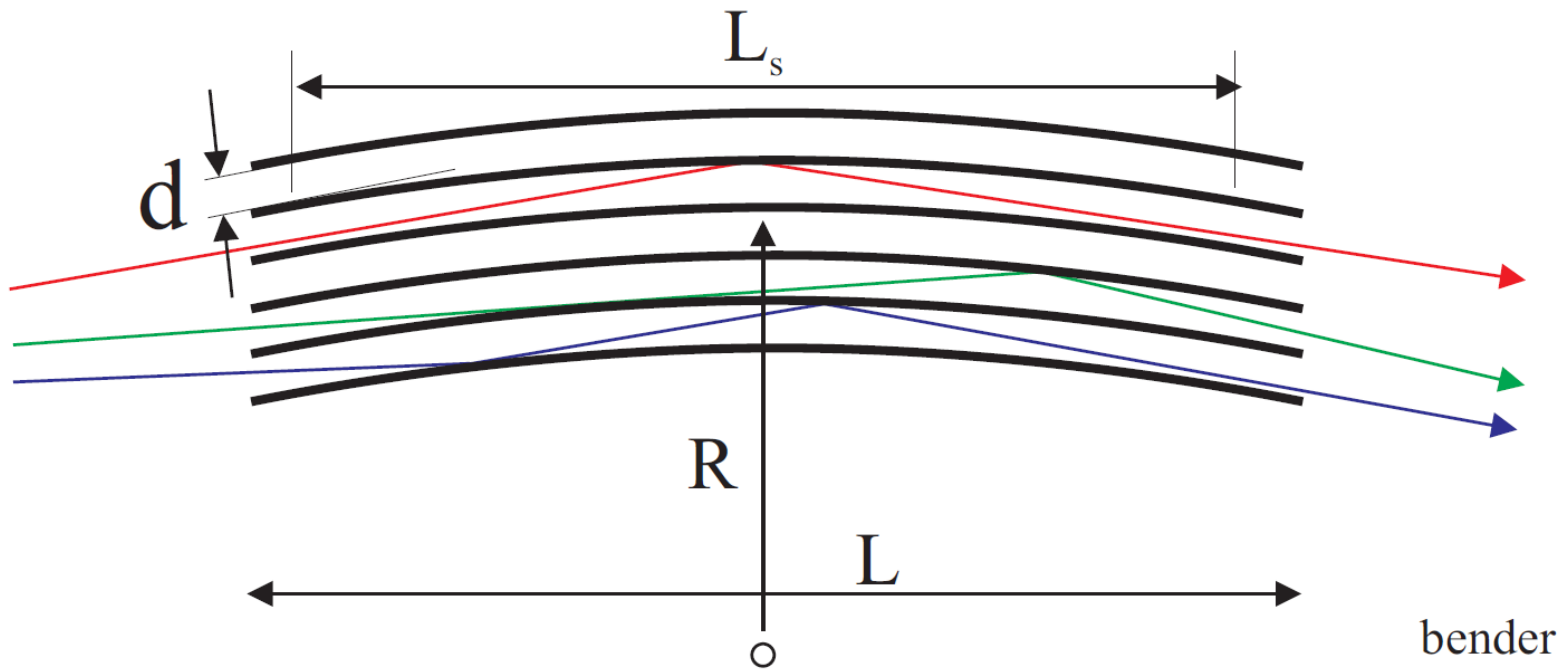
- maximum θ_c : $m = 5.5$
- $P > 99\%$

Fe/Si-Supermirror: Reflect and Polarize

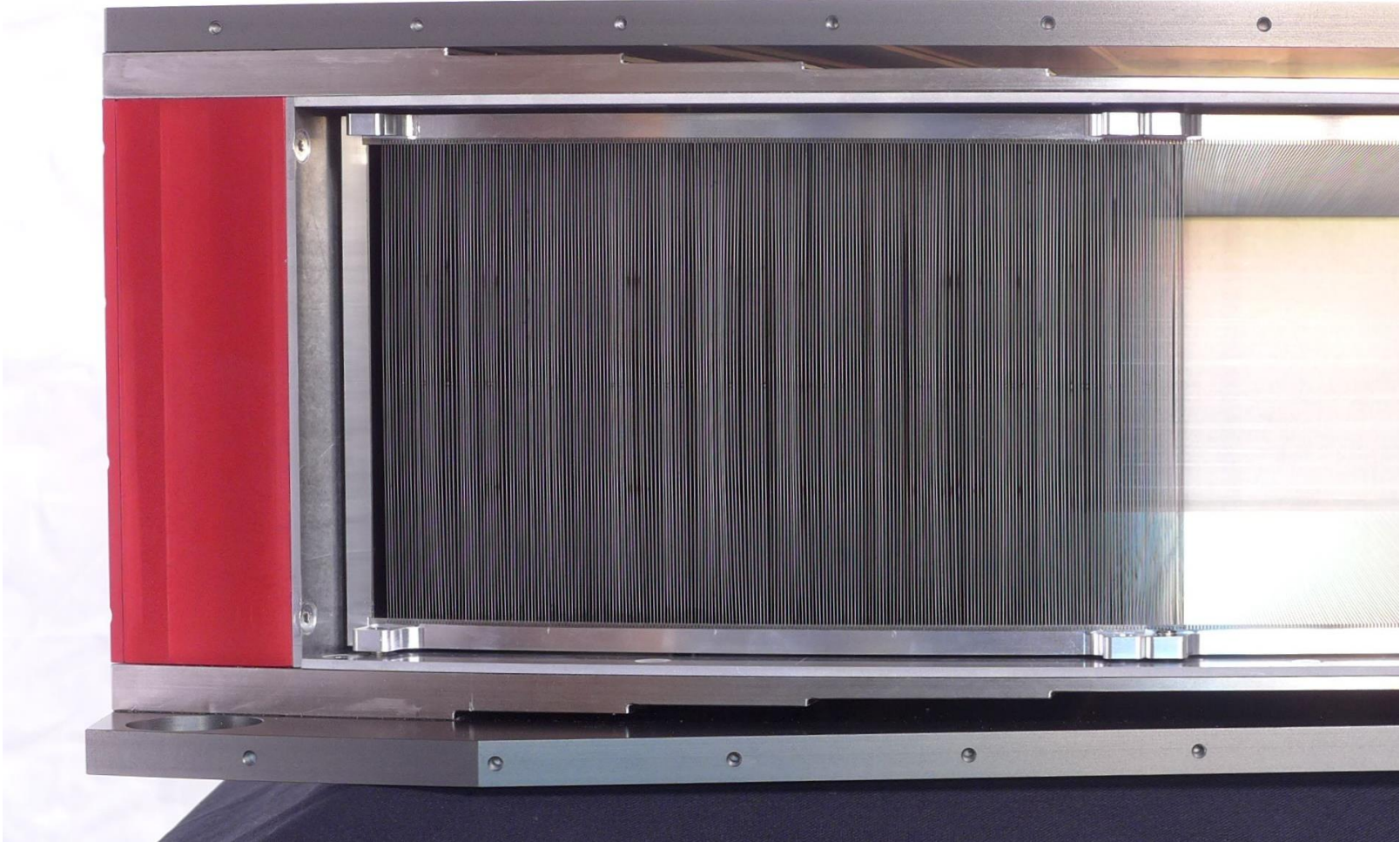


- $m = 5.5$
- $P > 99\%$

Polarizing Bender



Large Area Analyzers

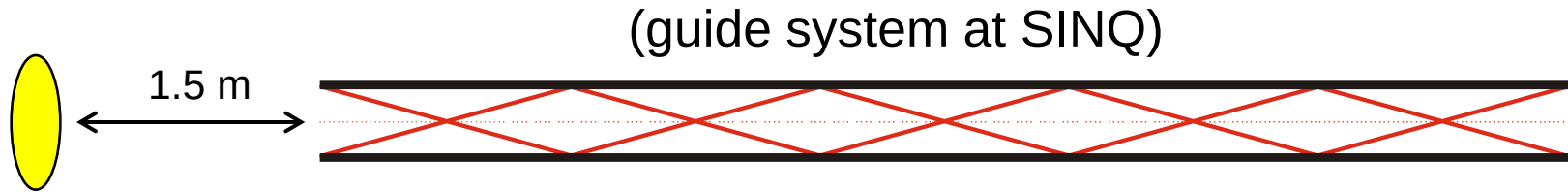


Thermal ToF: POLANO @ J-PARC

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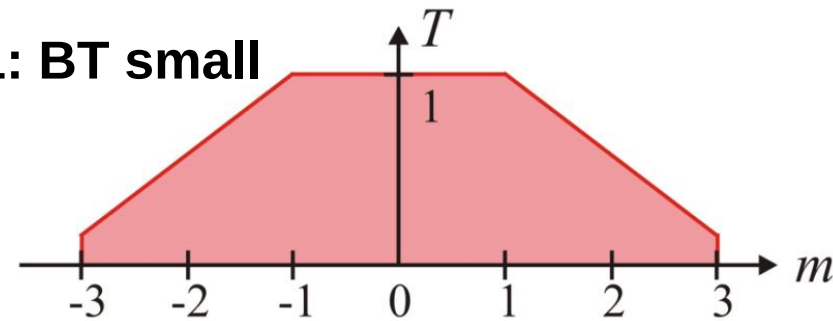
Brilliance Transfer: Standard vs. Elliptic Guides



drawbacks:

- non-compact phase space
- illumination losses
- large entrance $\rightarrow$ large background

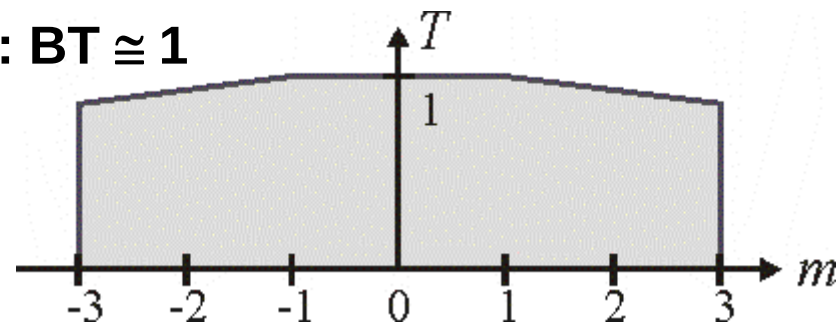
$n \gg 1$: BT small



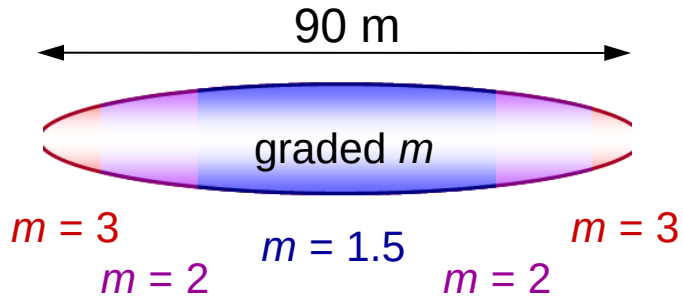
Advantages:

- compact phase space (tails reduced)
- no illumination losses (if ...)
- smaller moderator $\rightarrow$ lower background

$n \cong 2$: BT $\cong 1$

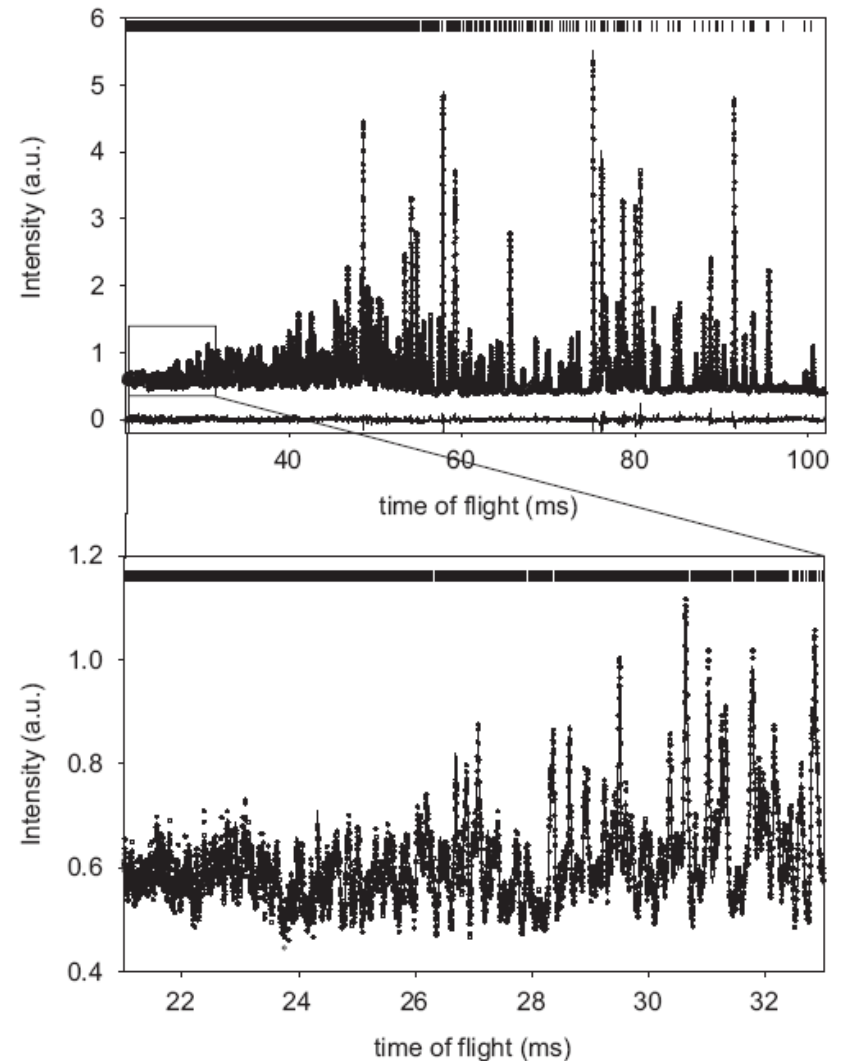
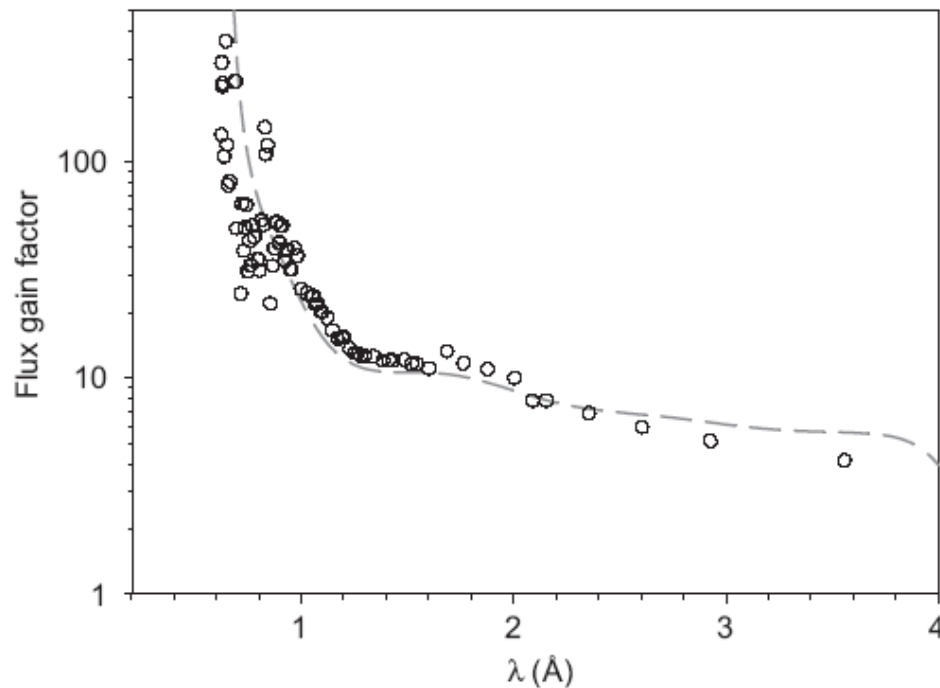


HRPD @ ISIS: Deuterated Benzene C_6D_6

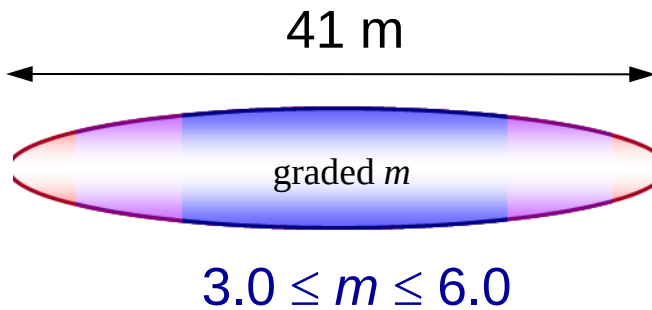


truly curved

designed: 2006

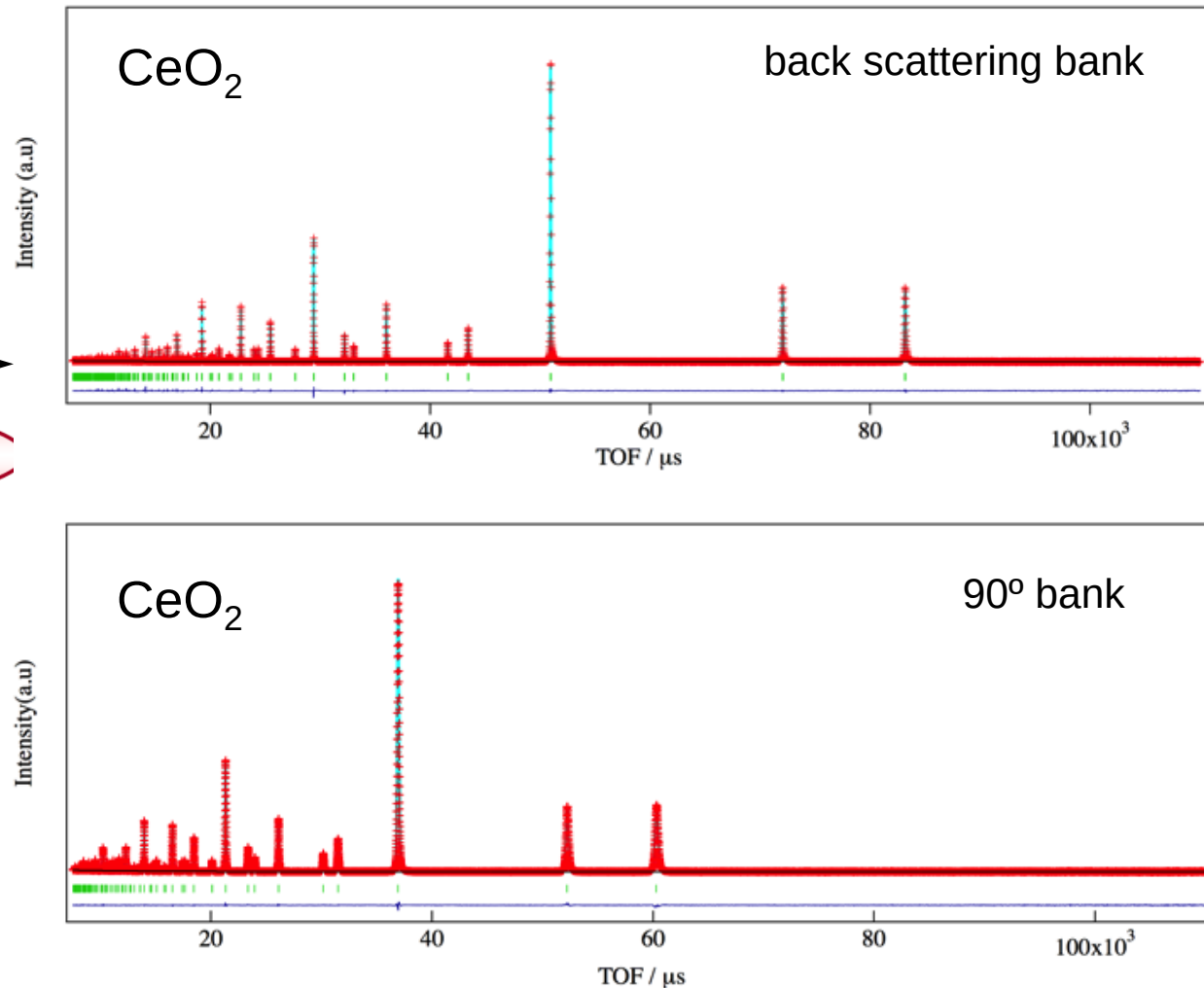


SPICA @ J-PARC: Diffraction from CeO_2



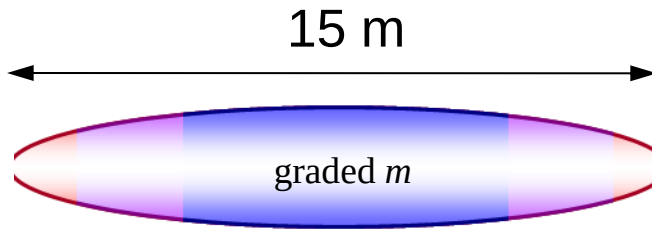
designed 2009

truly curved



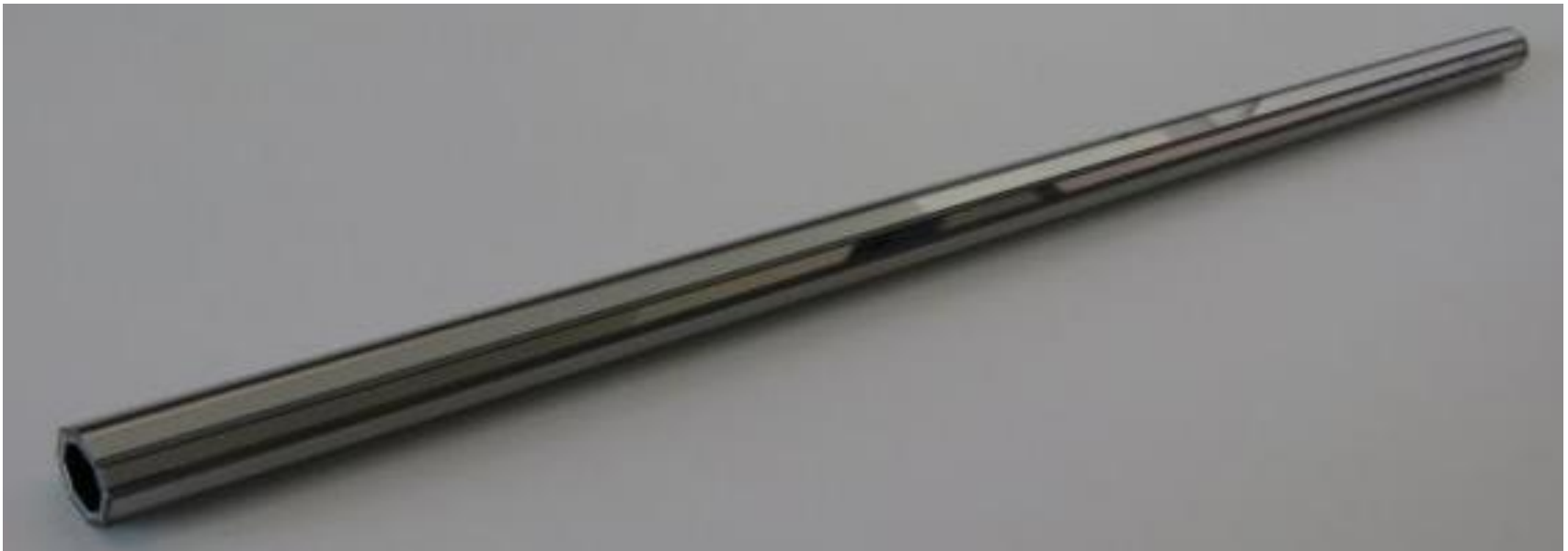
M. Yonemura, K. Mori, T. Kamiyama, T. Fukunaga, S. Torii, M. Nagao, Y. Ishikawa, Y. Onodera, and D.S. Adipranoto, SPICA_Proceeding_20130723v0TK1

POWTEX @ FRM-II: Octahedral-Elliptic Guide



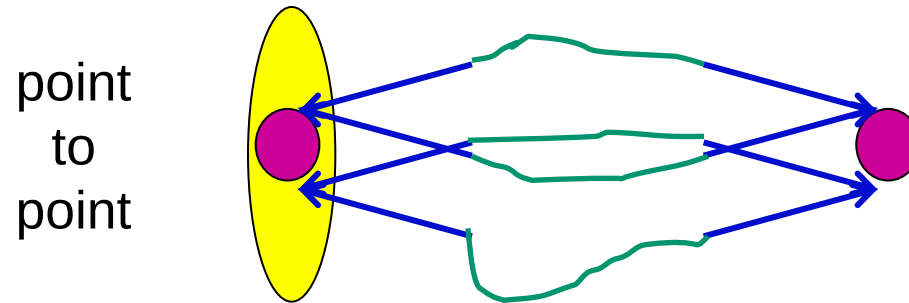
$$2.0 \leq m \leq 5.0$$

designed 2010

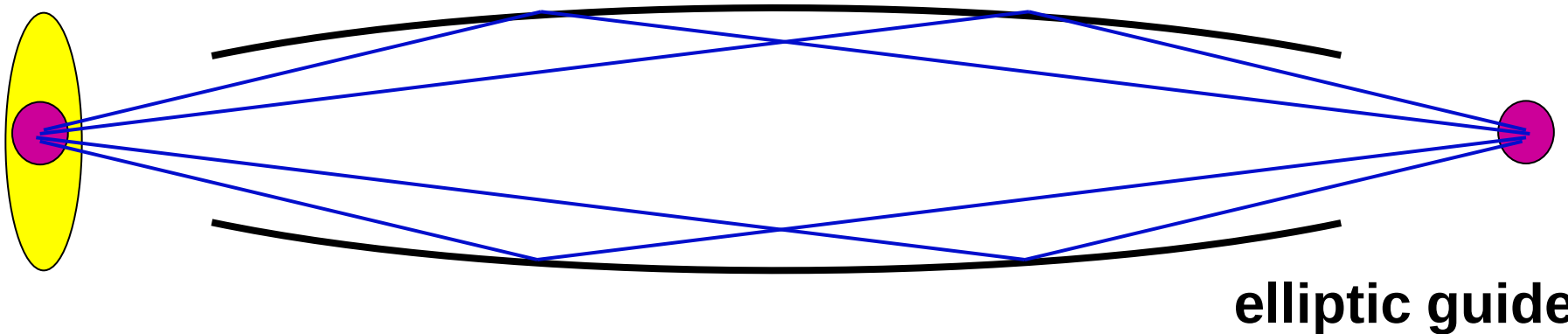


Brilliance Transfer with Elliptic Guides

from the idea:



to the realization:



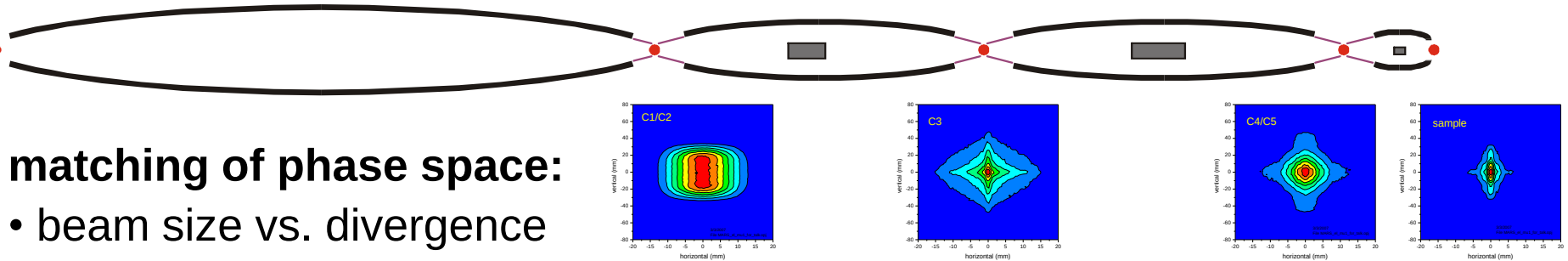
C. Schanzer et al., Nucl. Instr. Meth. A **529**, 63 (2004)

performance:

- brilliance transfer up to 90%: almost all useful neutrons transported
(K. H. Kleno et al., Nucl. Instr. Meth. A 696, 75 (2012))

Fooling Around With Elliptic Guides

Reduction of background / equalize path lengths / reduce chopper size:

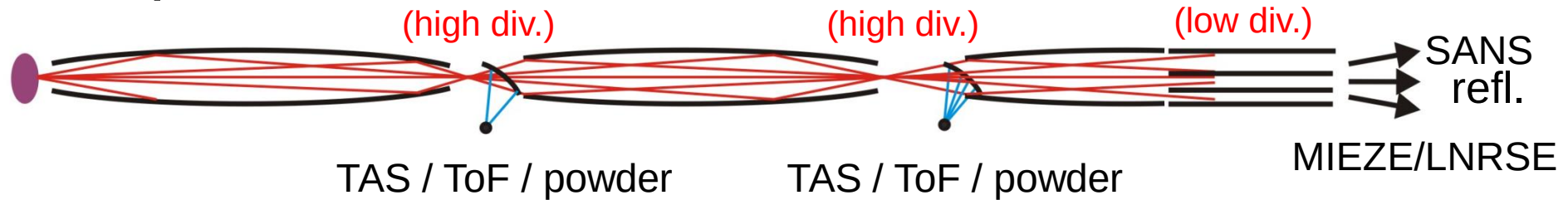


matching of phase space:

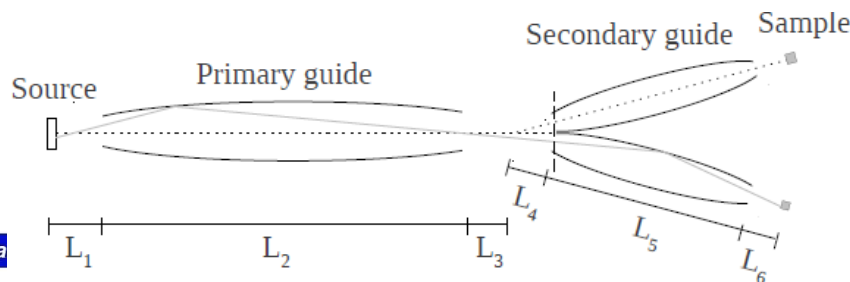
- beam size vs. divergence
- flight time is constant

P. Böni, Nuclear Instr. Meth. A **586** (2008) 1

Multiple use of beams:



Neutron guide-split: guide bundle concept for elliptical guides



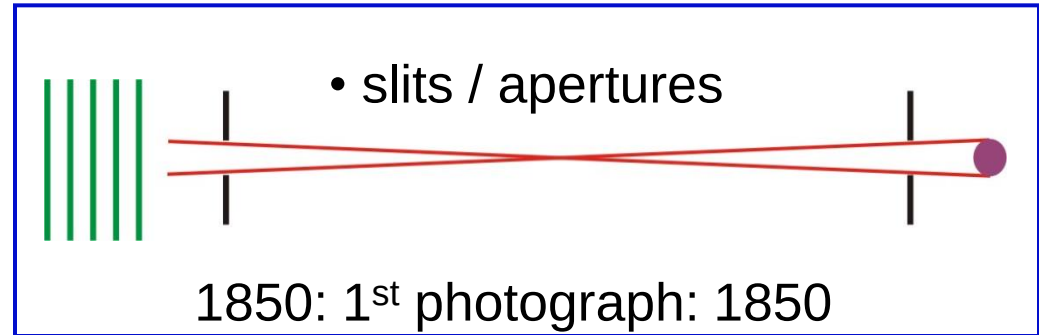
S. L. Holm, K. Lefmann, K. Andersen et al., Nucl. Instr. Methods **782**, 1 (2015)

Content

- Introduction
- Supermirrors
- Transport
- **Focusing Optics**
- Montel Mirrors
- Beam Extraction
- Summary

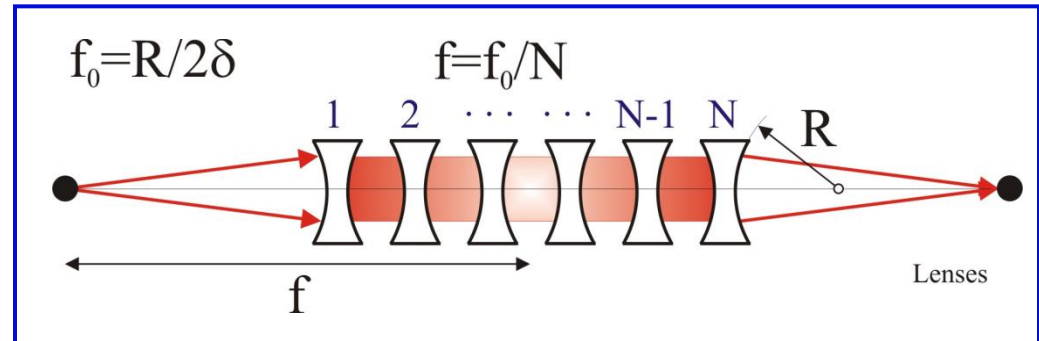
Focused Beams for Small Samples (1 - 30 mm)

- pin-hole camera:
(used for neutron scattering)

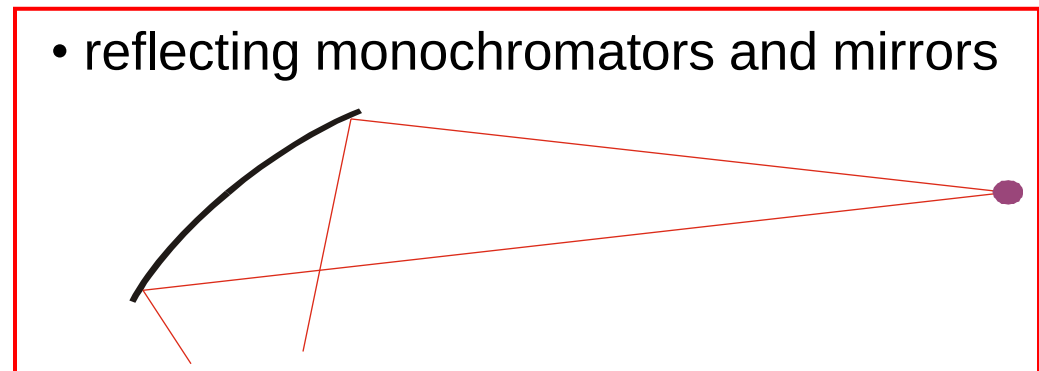


- lenses (comp. hexapoles):
(chromatic aberration)

M. Eskildsen et al., Nature **391**, 563 (1998)



- reflection optics:
(no chromatic aberration)



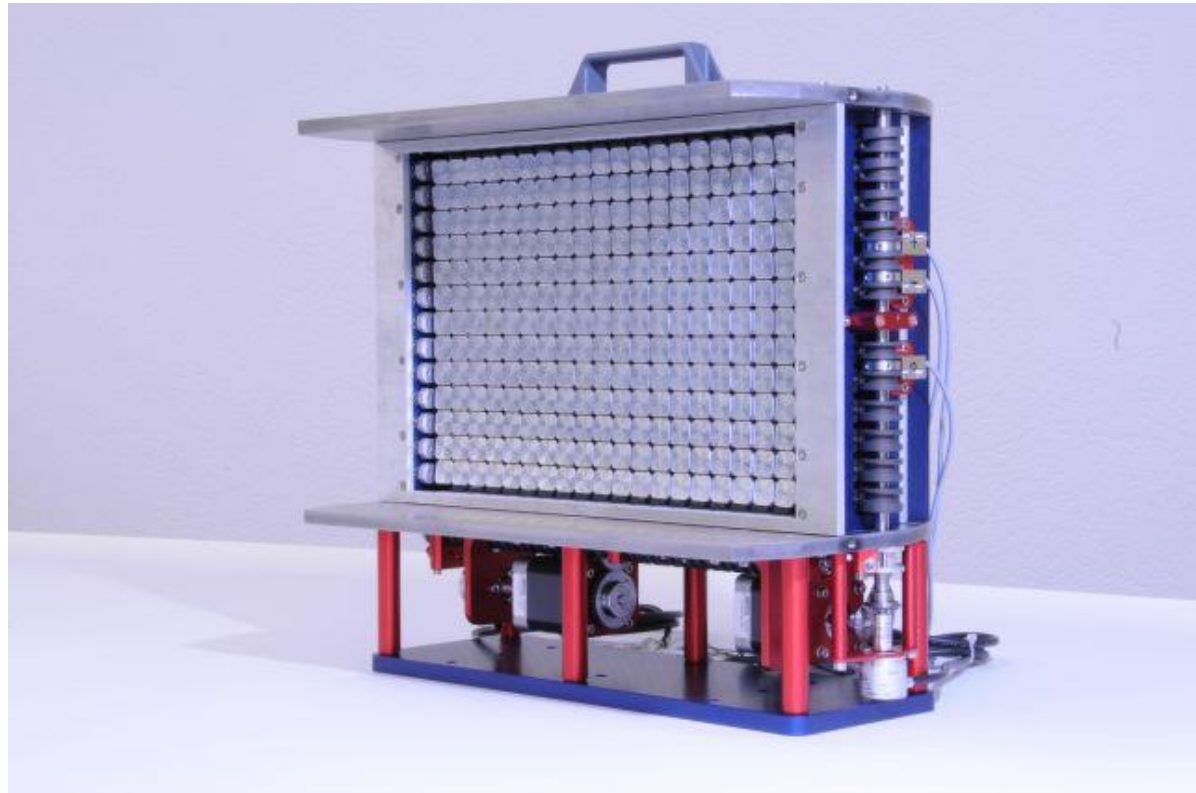
Focusing Monochromators

Focusing:

- Bragg reflection from curved monochromators
(W. Bührer, Nucl. Instr. Meth. A **338**, 44 (1994))
- instead of an explanation: KOMPASS @ FRM-II

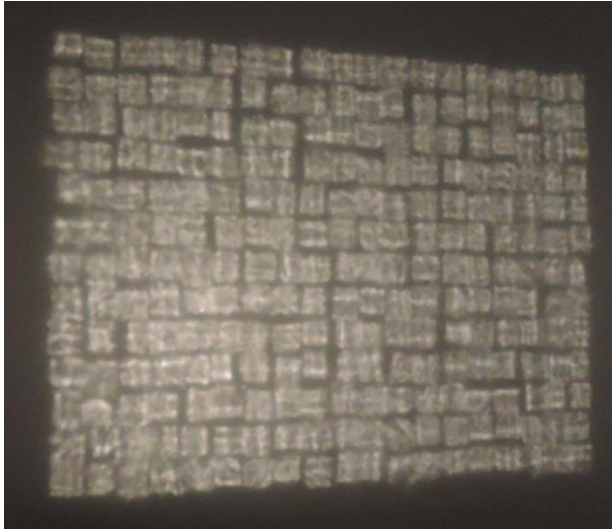
specification:

- area: $193 \times 275 \text{ mm}^2$
- 13 rows
- 19 columns
→ **247 monochromators**
- crystal size:
 $14 \times 14 \text{ mm}^2$



Visualization of Focusing Monochromator

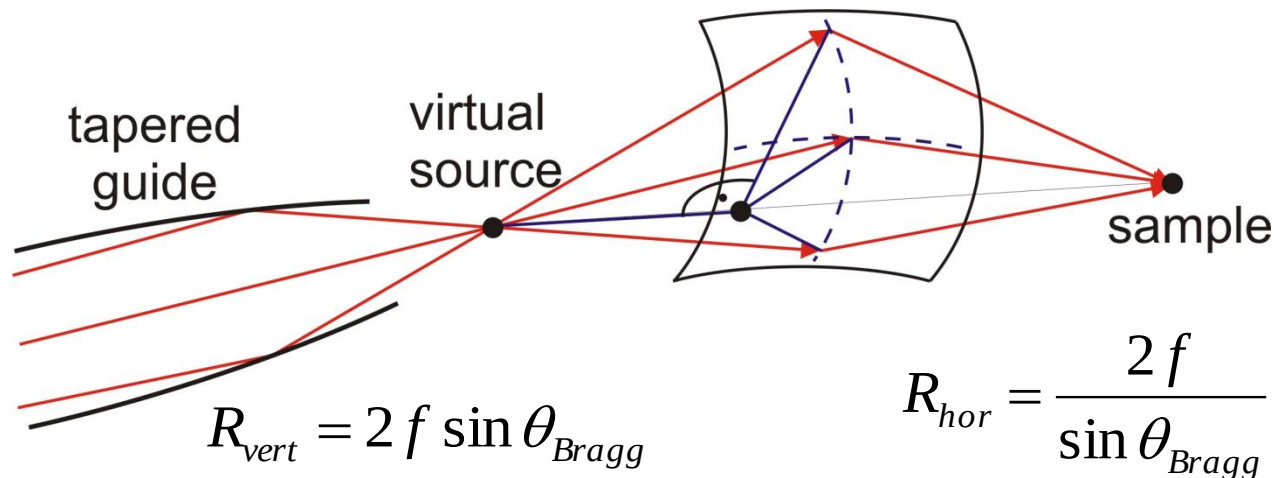
flat



vert./horiz. focusing



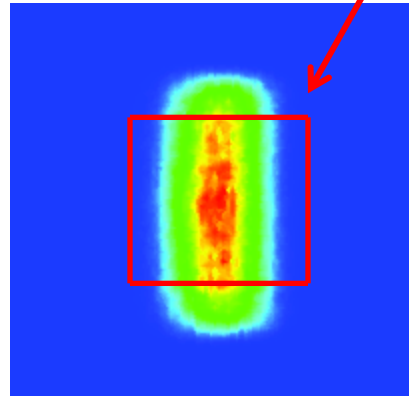
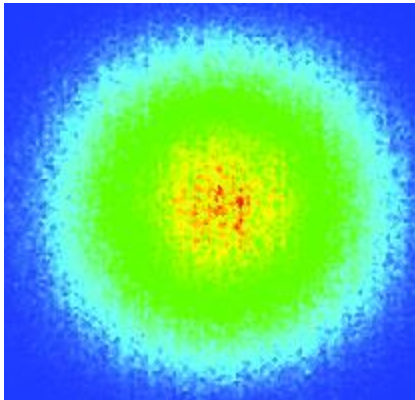
doubly foc.



Limits of Focusing Monochromator

Example: PANDA @ FRM-II

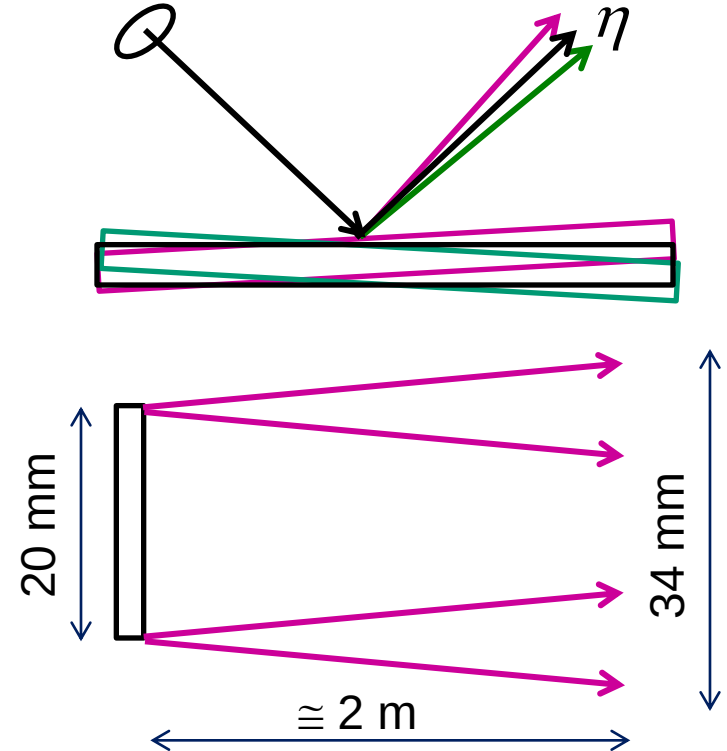
- crystal size: $20 \times 20 \text{ mm}^2$
- mosaic: $\eta = 0.5^\circ$



fwhm: $34 \times 34 \text{ mm}^2$ divergence: $2^\circ \times 5^\circ$

Drawbacks:

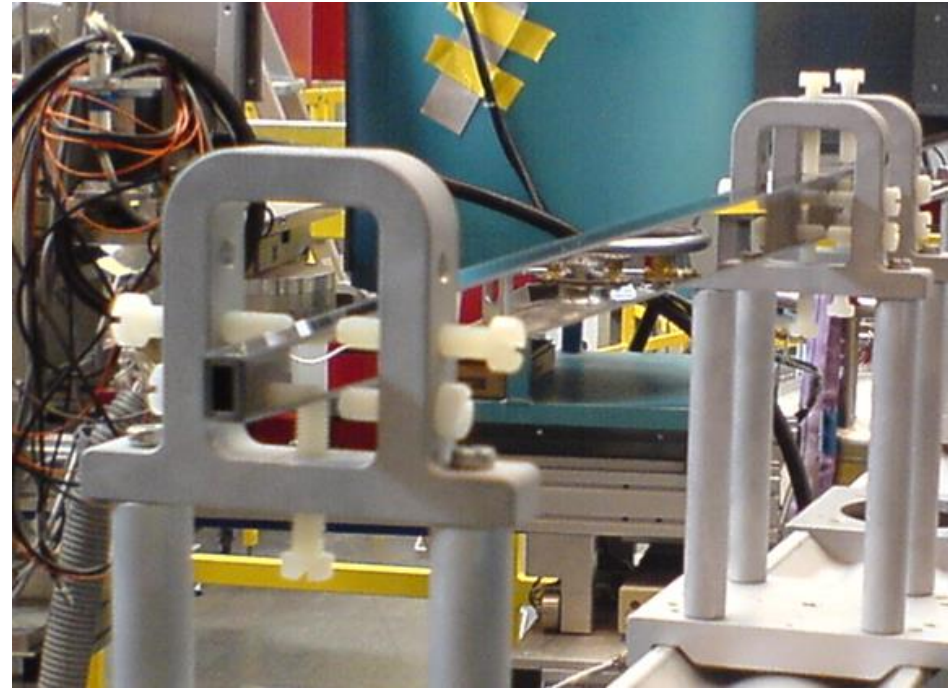
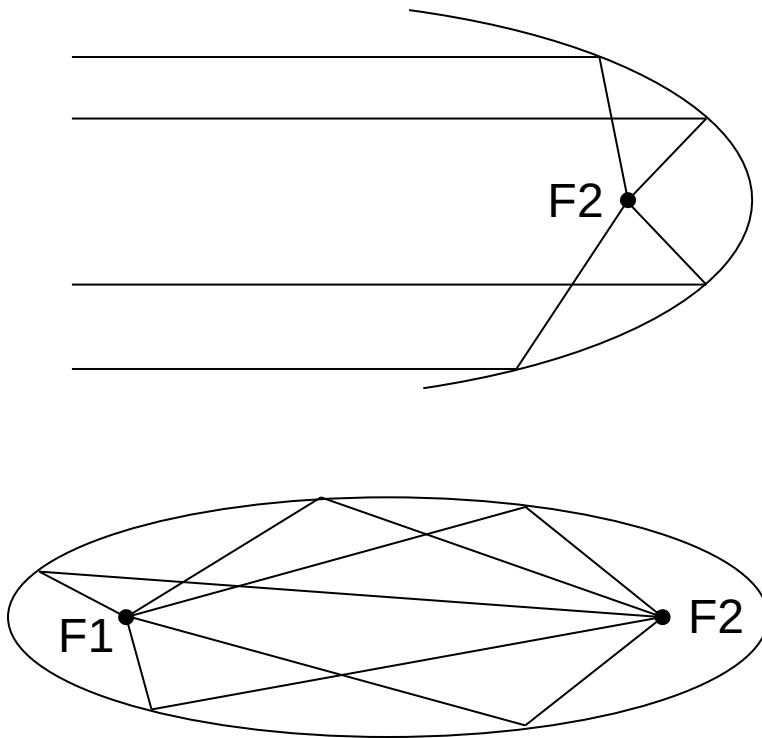
- beam still very large
- edges diffuse: slits/collimation required



Focusing Guides

Given:

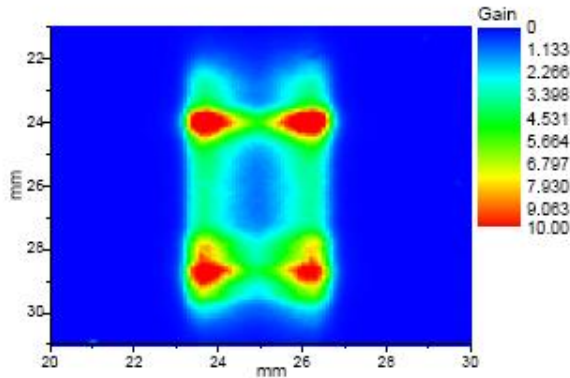
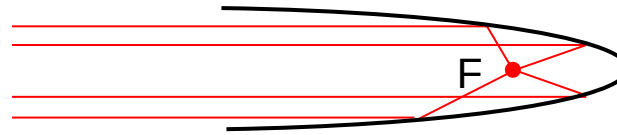
- beam line positioned at a conventional (straight) guide
- define beam size and divergence at sample $\rightarrow I = \eta \cdot A \cdot \Delta\lambda \cdot \Omega \cdot \Psi$
- design: parabolic / elliptic



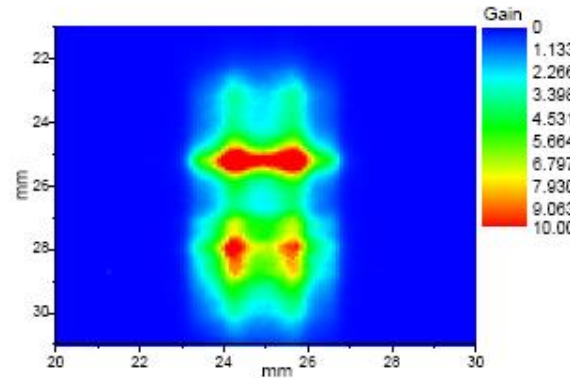
set-up @ MORPHEUS @ SINQ

Parabolic Focusing at 3 Å

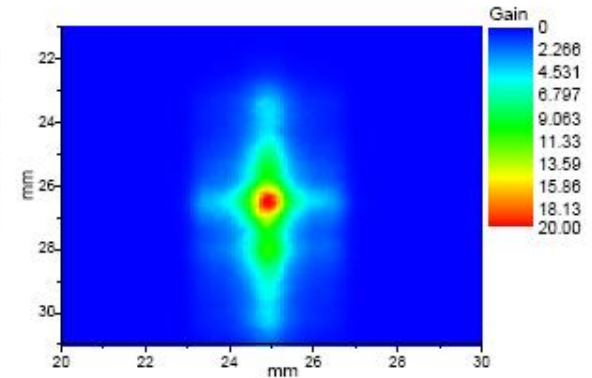
Wavelength: 3 Å



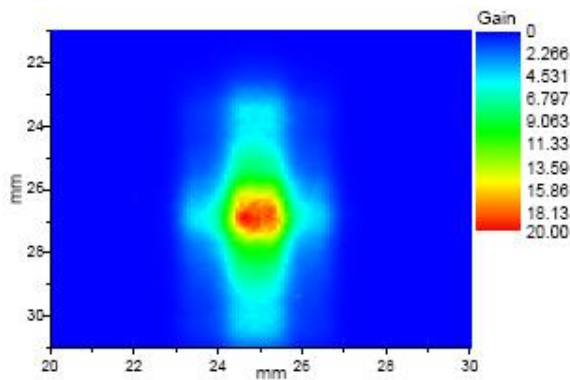
Distance: 0 mm



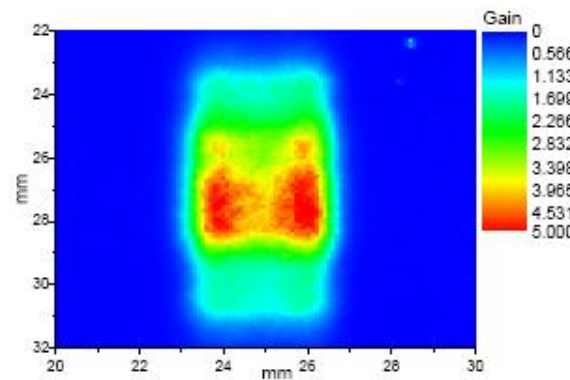
40 mm



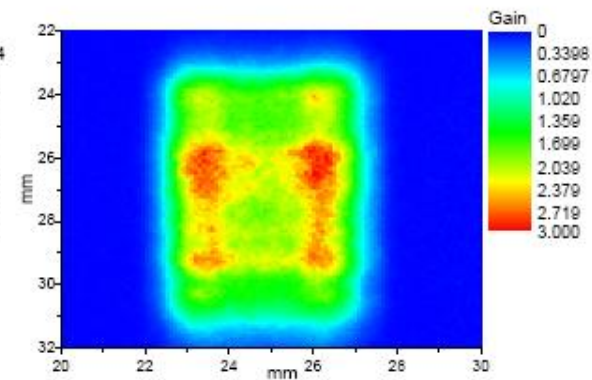
80 mm



Distance: 100 mm



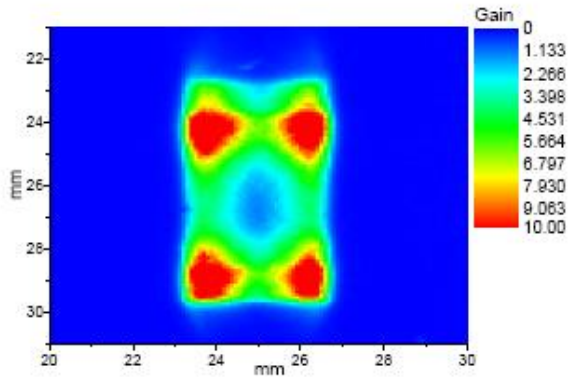
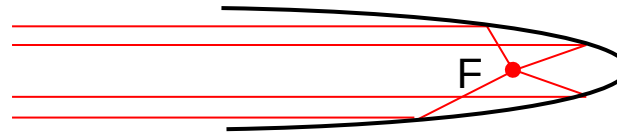
150 mm



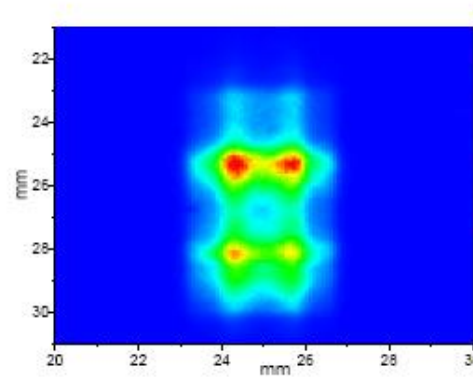
200 mm

Parabolic Focusing at 3 Å

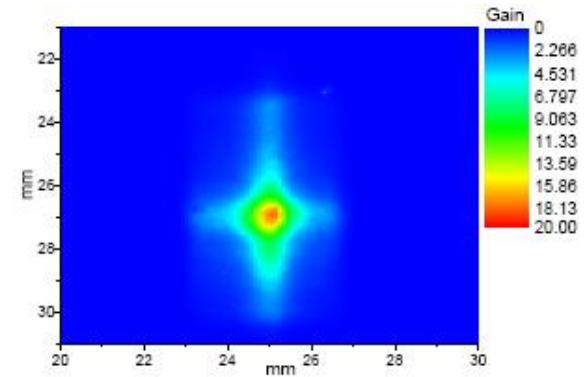
Wavelength: 6 Å



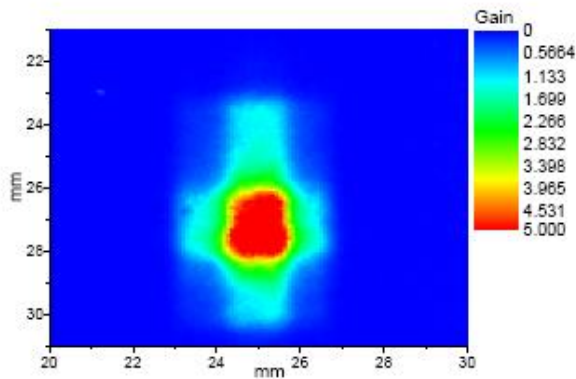
Distance: 0 mm



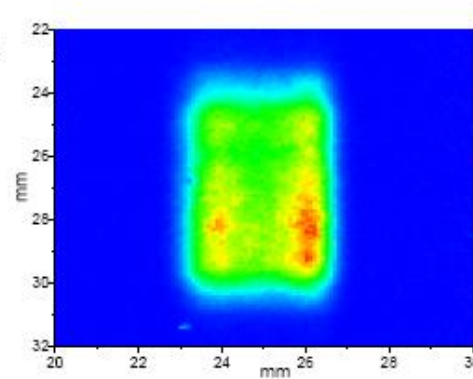
40 mm



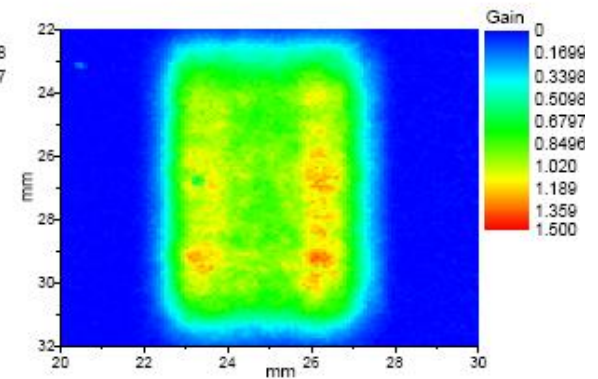
80 mm



Distance: 100 mm



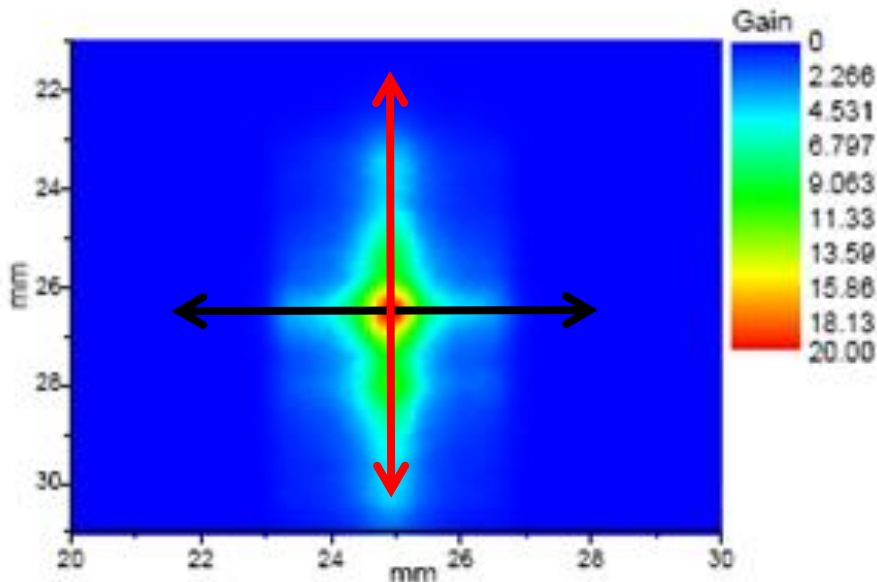
150 mm



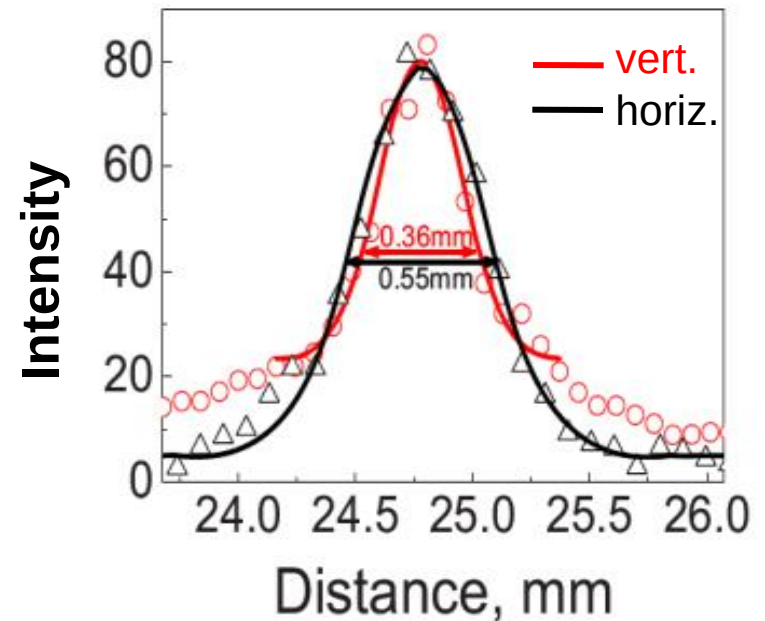
200 mm

Beam Size for Parabolic Focusing

spatial distribution of intensity:



width of beam:

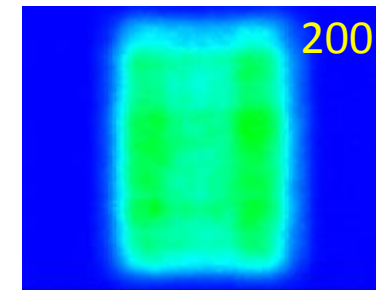
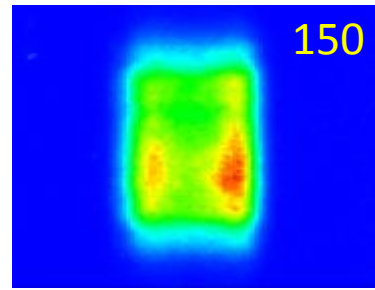
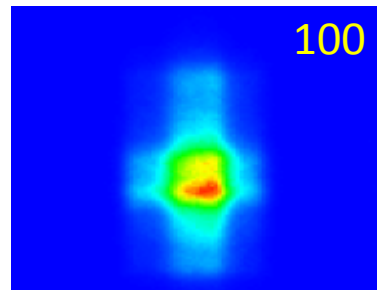
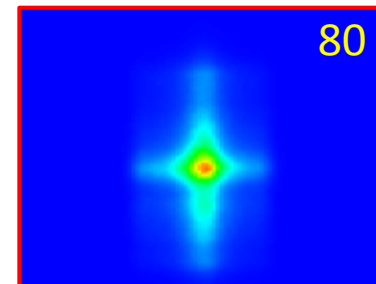
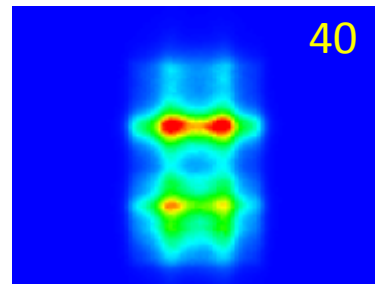
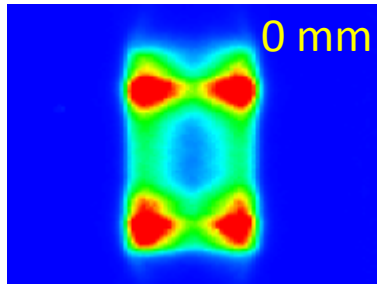


→ remove wings by masking direct beam

result: sub-millimeter beam size

Experiment versus Monte Carlo

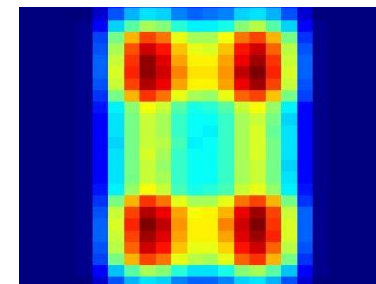
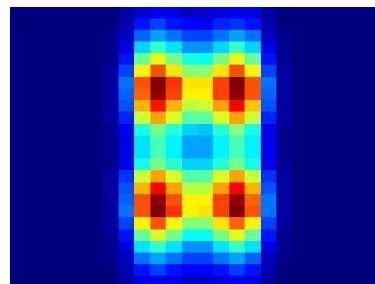
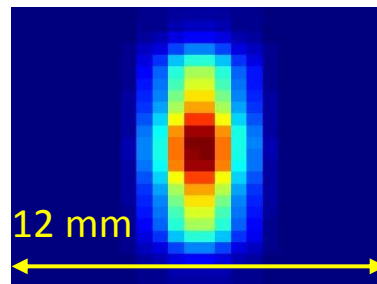
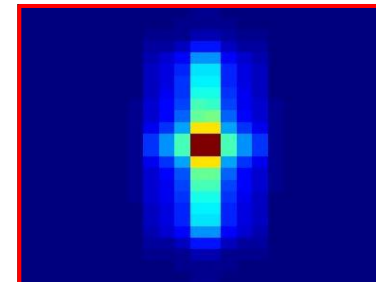
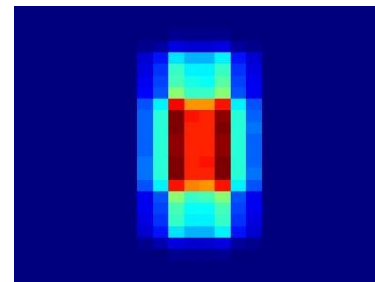
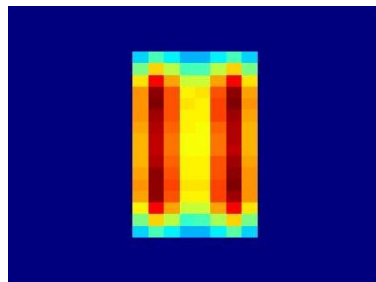
experiment



Focusing tube:

- ↪ $L = 500$ mm
- ↪ $W_{in} = 10.6$ mm
- ↪ $H_{in} = 21.2$ mm
- ↪ $W_{out} = 4.0$ mm
- ↪ $H_{out} = 8.0$ mm
- ↪ $f = 80$ mm
- ↪ $m = 3$
- ↪ $R = 73\%$

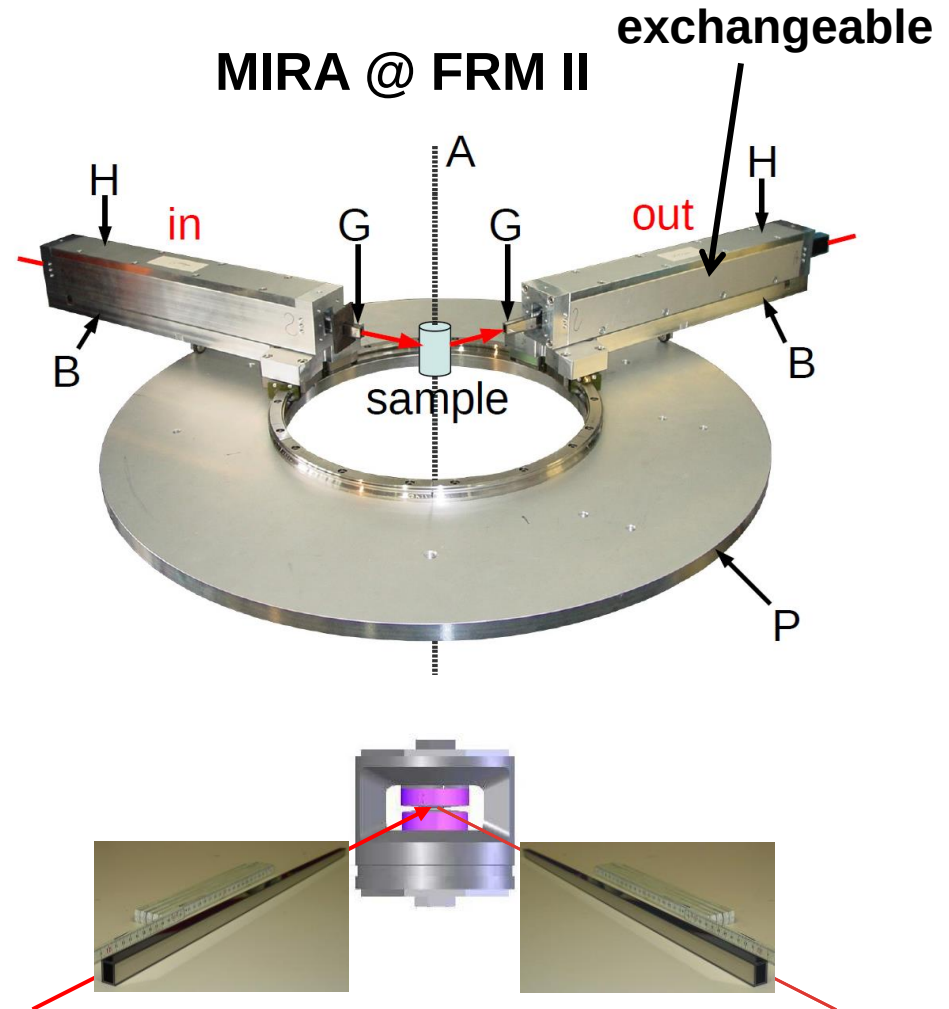
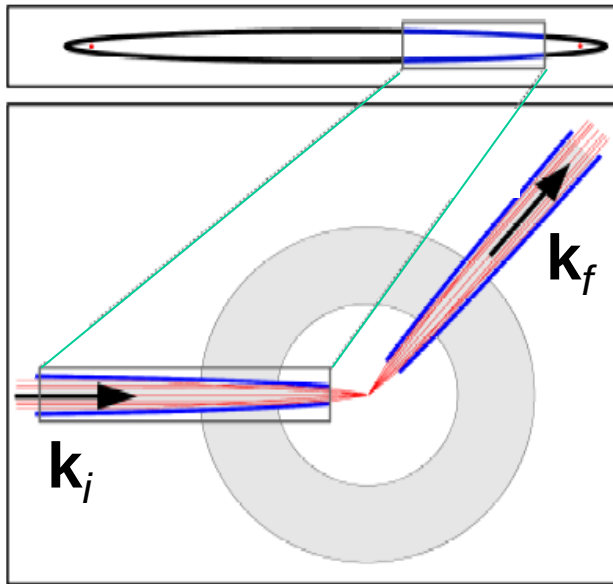
simulation



Set-up:

- ↪ $\lambda = 4$ Å
- ↪ hor. div.: 15'
- ↪ vert. div.: 60'

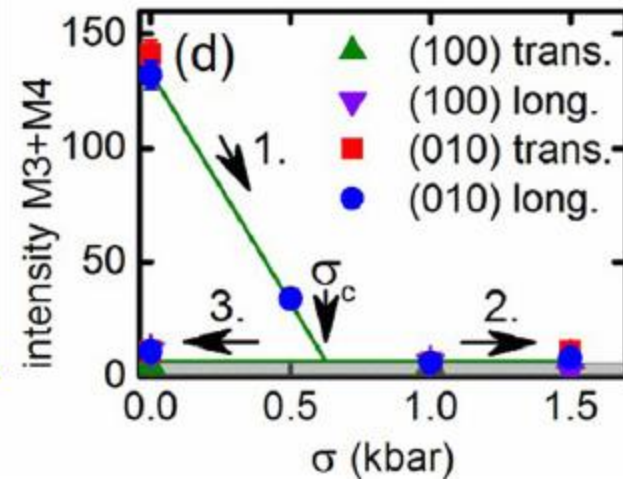
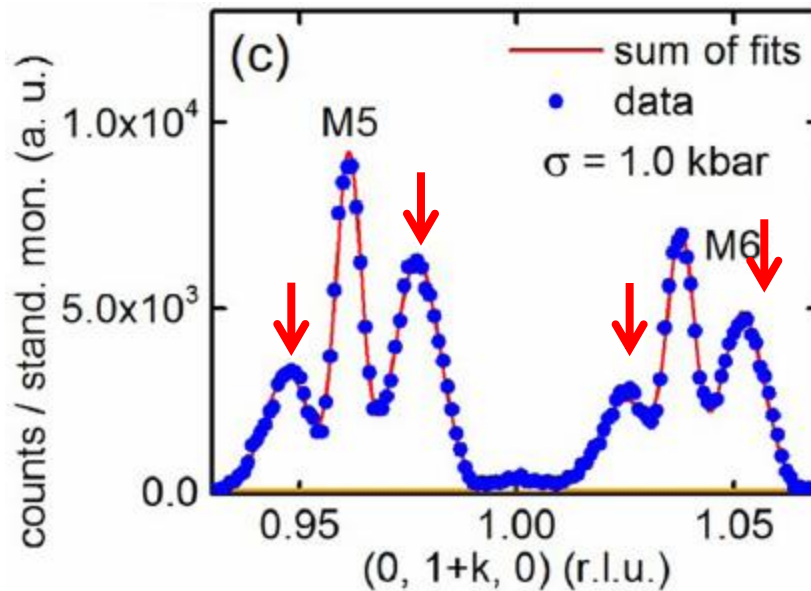
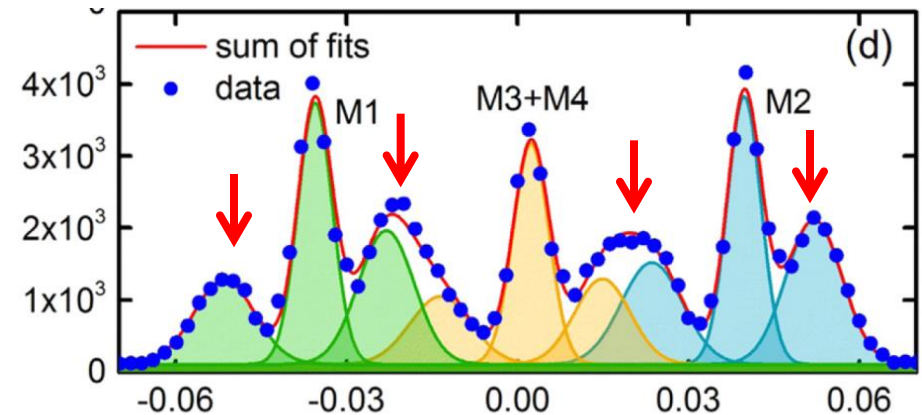
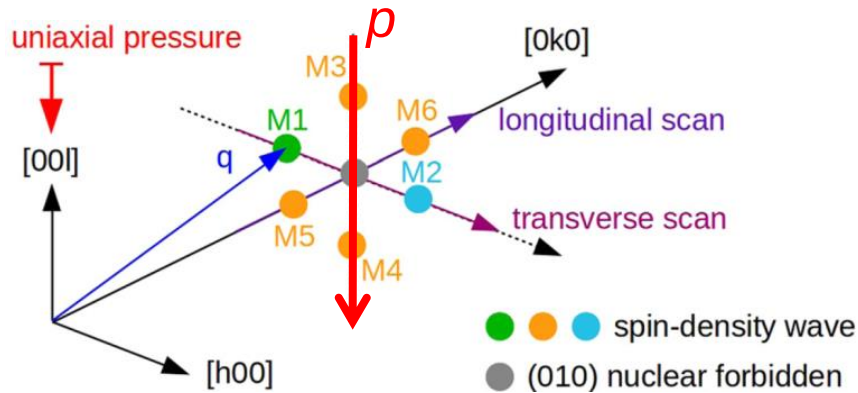
Focusing Set-Up Using Parabolic Guides



- focusing before
- and
- defocusing after sample

Implementation at existing beam lines possible

Domain Population in Cr under Uniaxial Stress



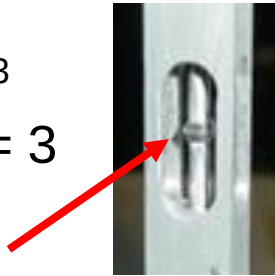
technology: $G = 4$

science: investigate tri-critical point

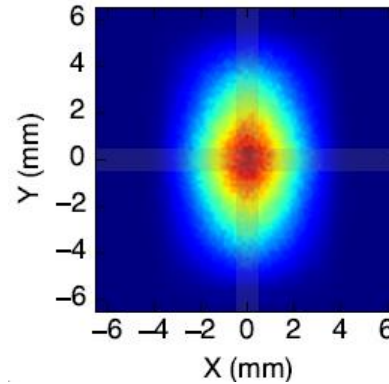
Focusing and Inelastic Neutron Scattering

Phonons in Pb

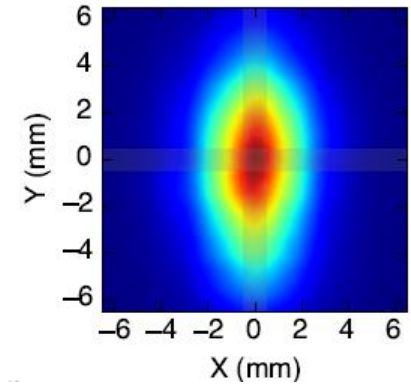
- sample: $2 \times 2 \times 2 \text{ mm}^3$
- focusing guides: $m = 3$



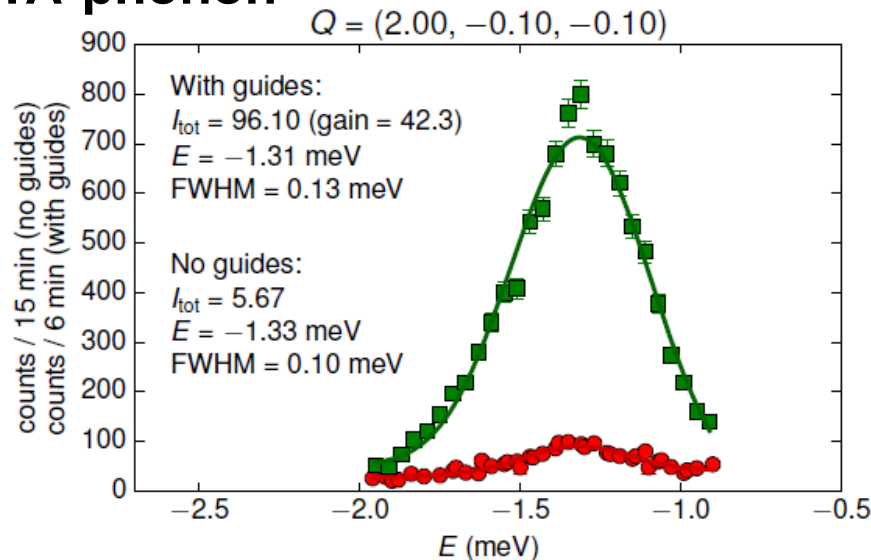
McStas simulation



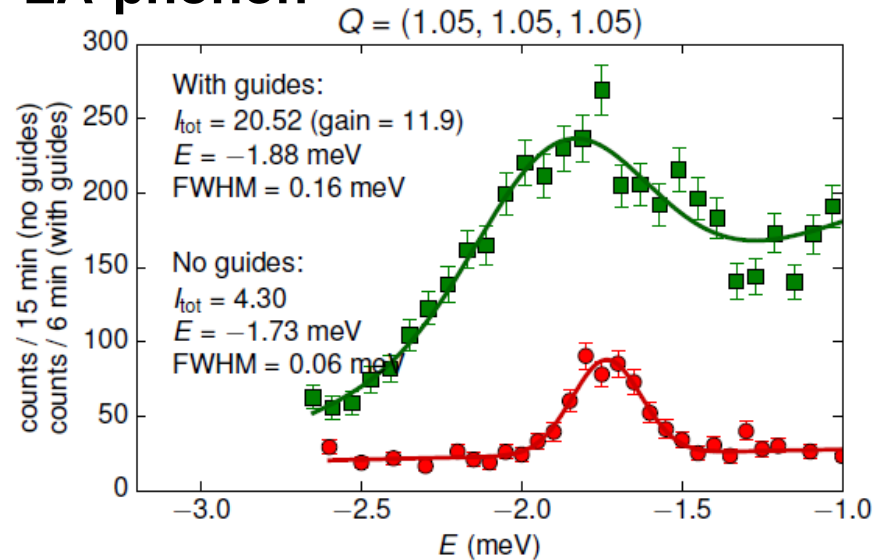
Measurement



TA-phonon



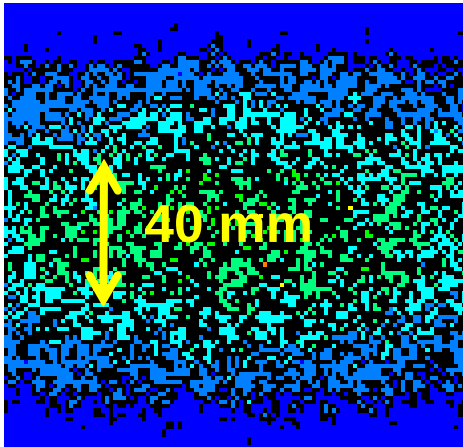
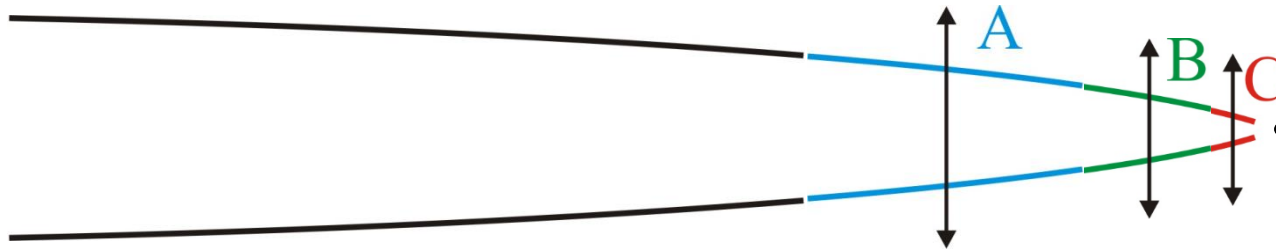
LA-phonon



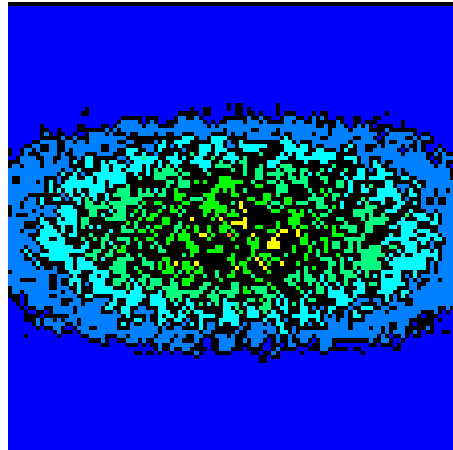
technology: $G = 42$ (pred. 2003)%

science: investigation of QPTs, etc.

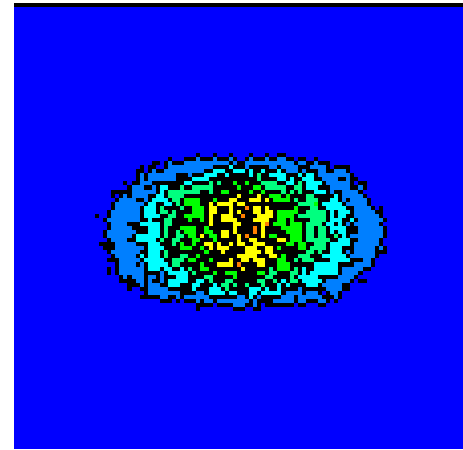
Focusing: Adaption of Beam Size



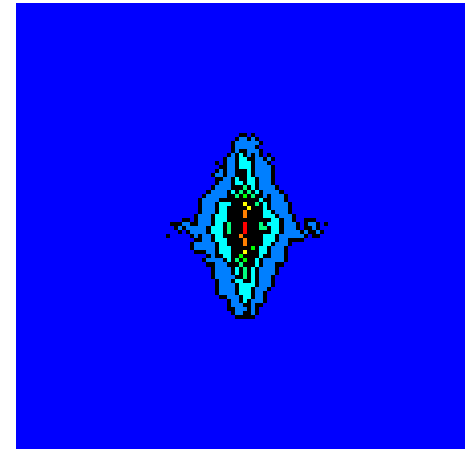
$f_{out} = 1.2 \text{ m}$



$f_{out} = 0.5 \text{ m}$



$f_{out} = 0.2 \text{ m}$

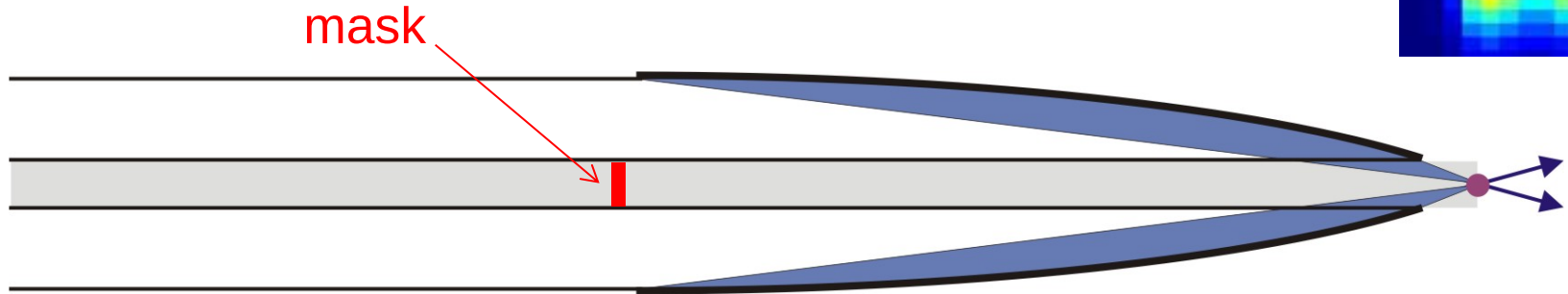
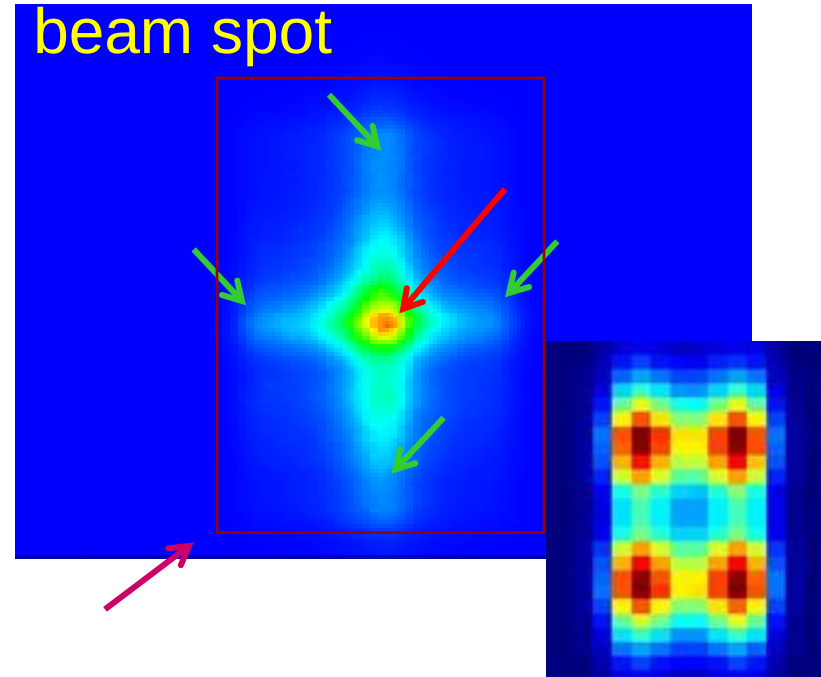
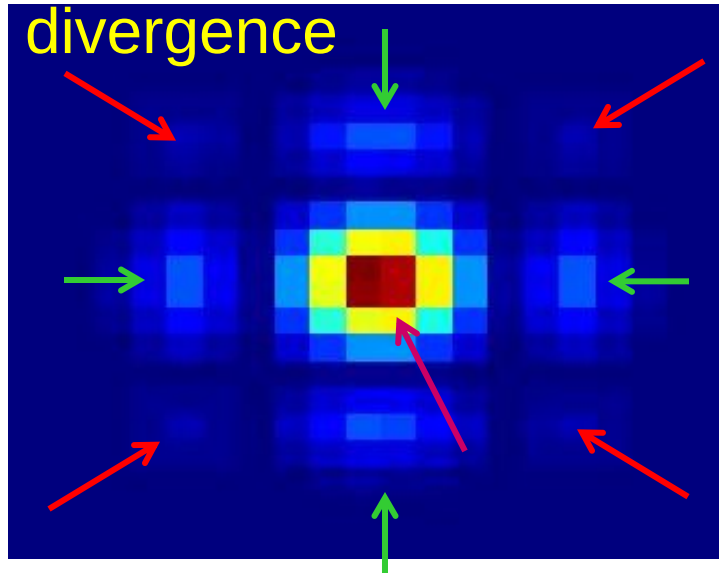


$f_{out} = 0.1 \text{ m}$

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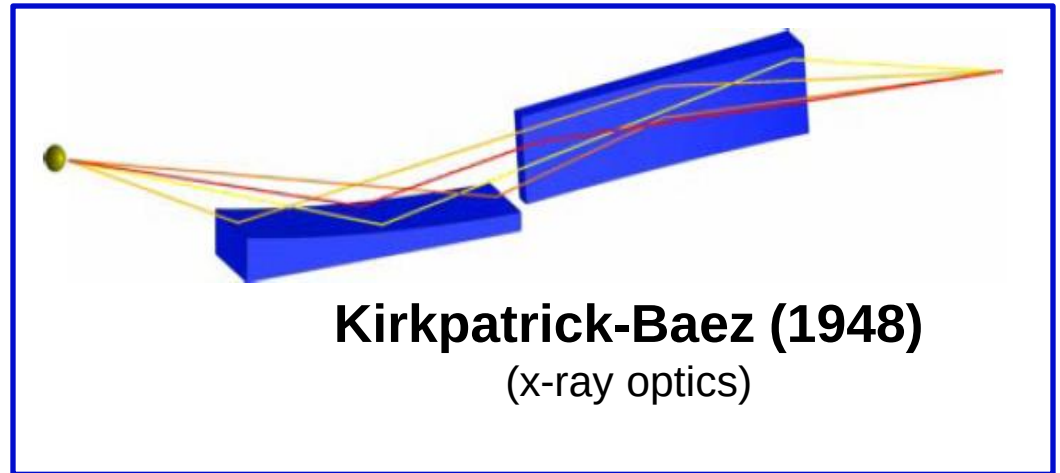
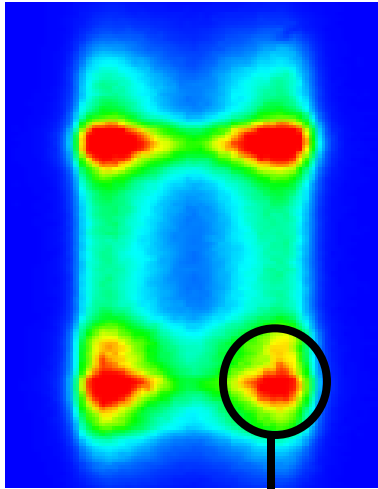
Divergence Is Inhomogeneous



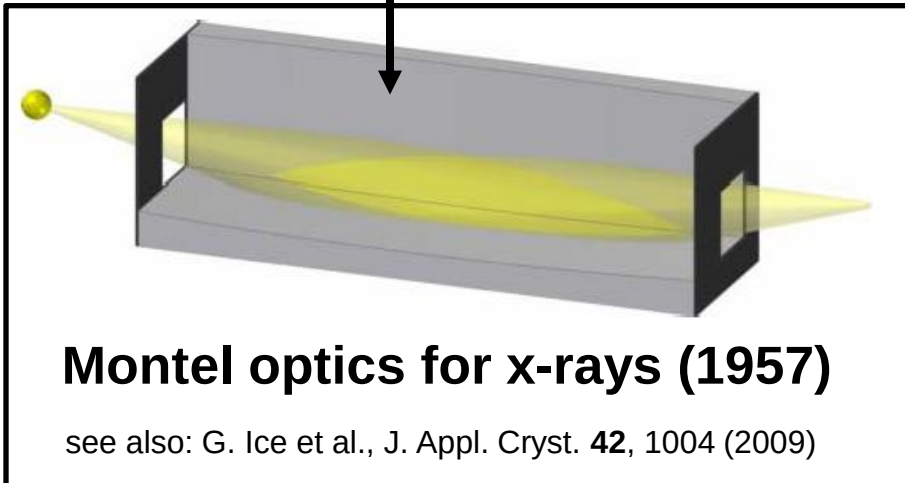
↳ long guide → more homogeneous divergence

↳ mask direct beam: wings reduced

Guides → Montel Optics



Kirkpatrick-Baez (1948)
(x-ray optics)



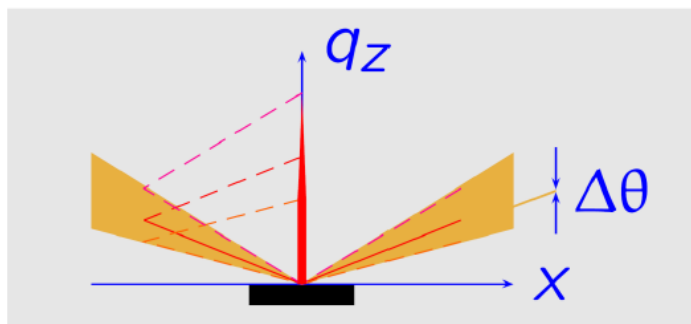
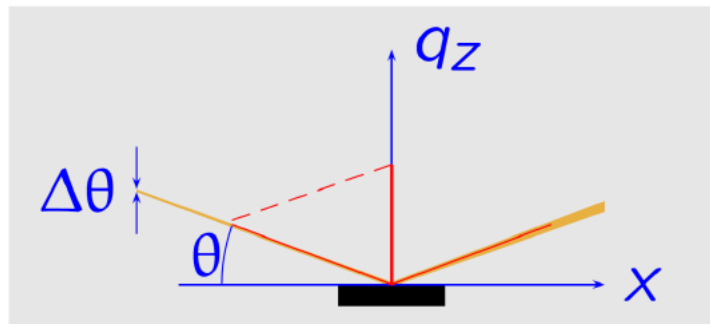
Montel optics for x-rays (1957)

see also: G. Ice et al., J. Appl. Cryst. **42**, 1004 (2009)

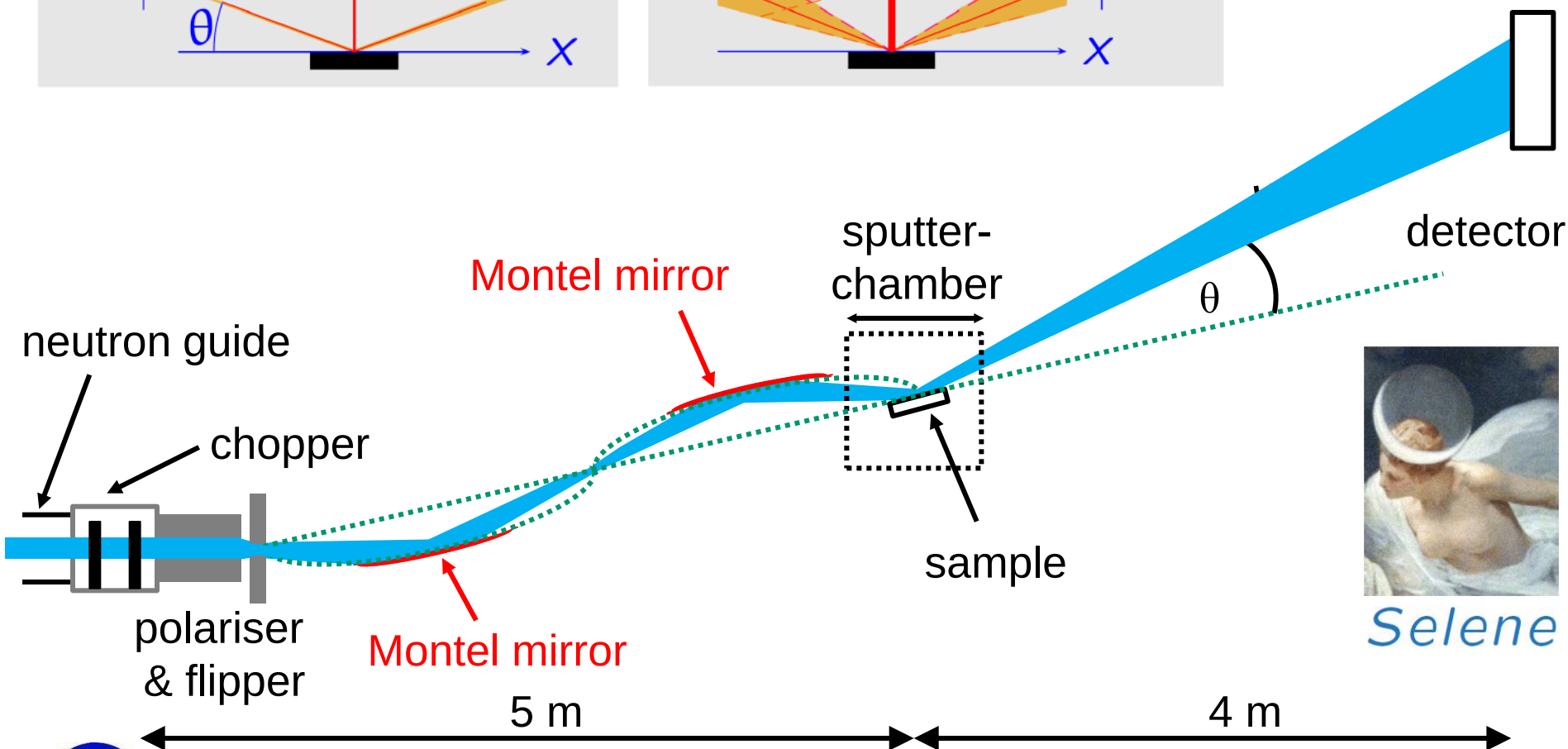
next
step:



Montel Mirrors for Reflectometry: AMOR @ SINQ



Idea:
J. Stahn, PSI

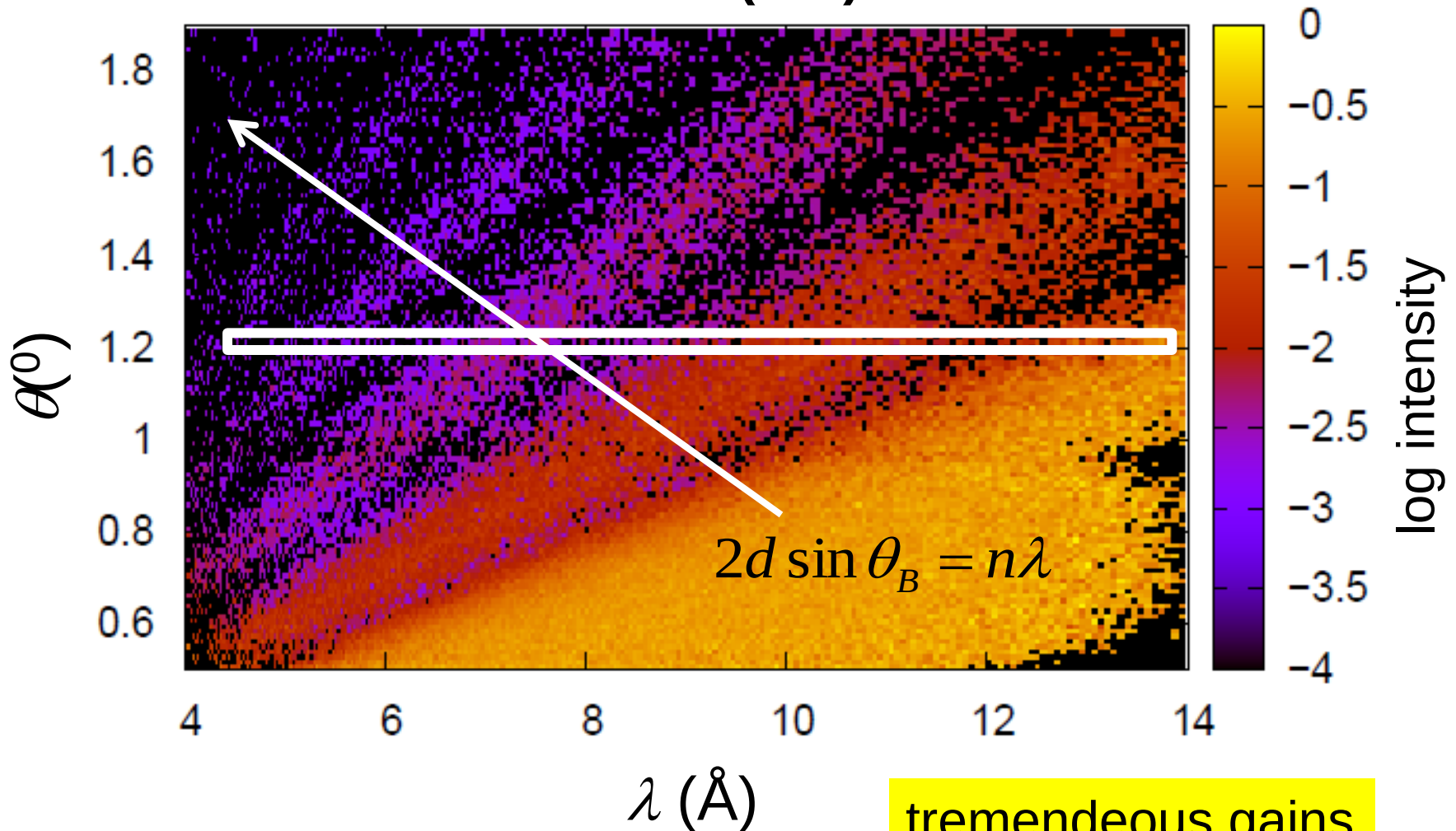


Installation of *In-situ* Chamber on AMOR

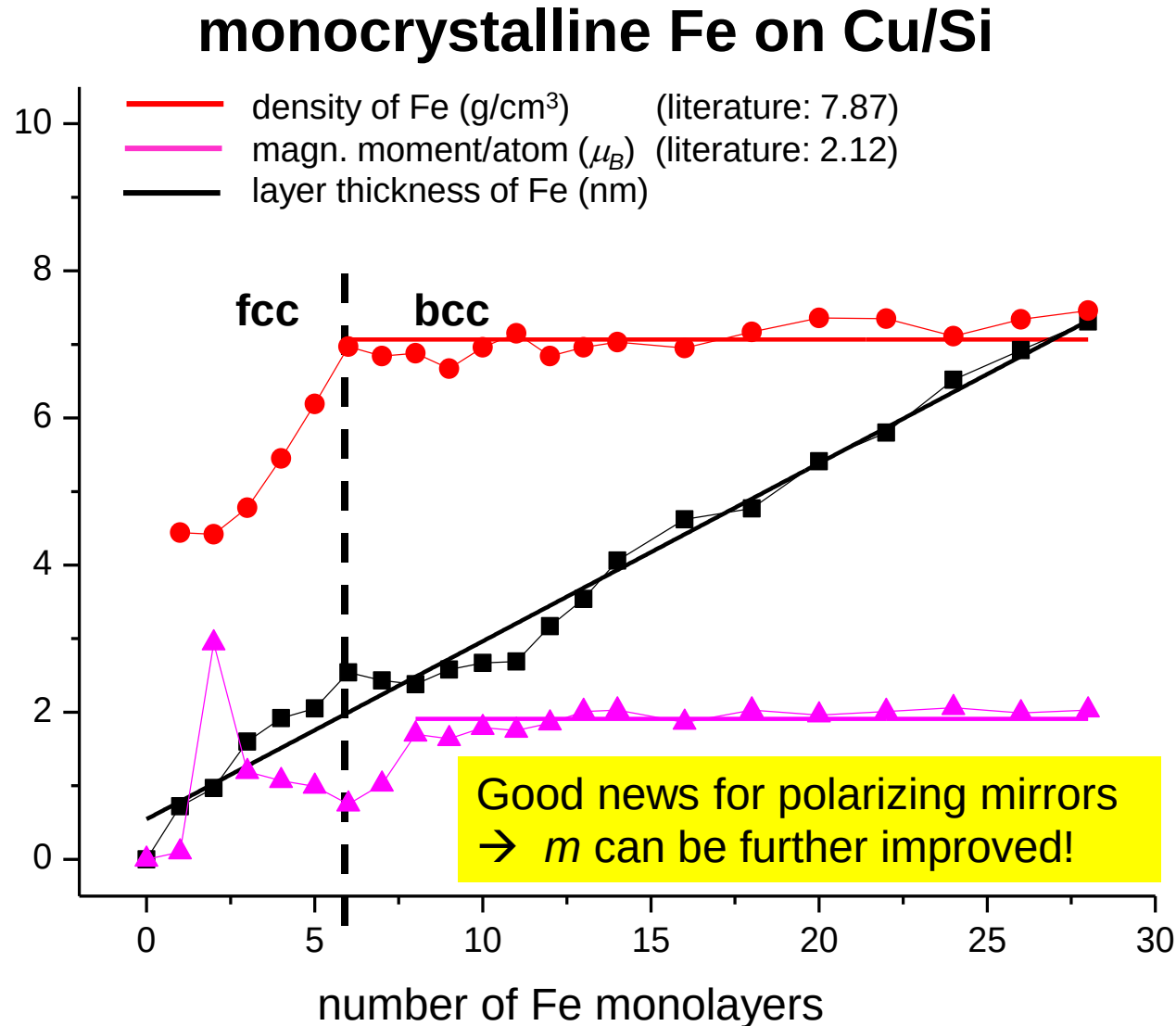
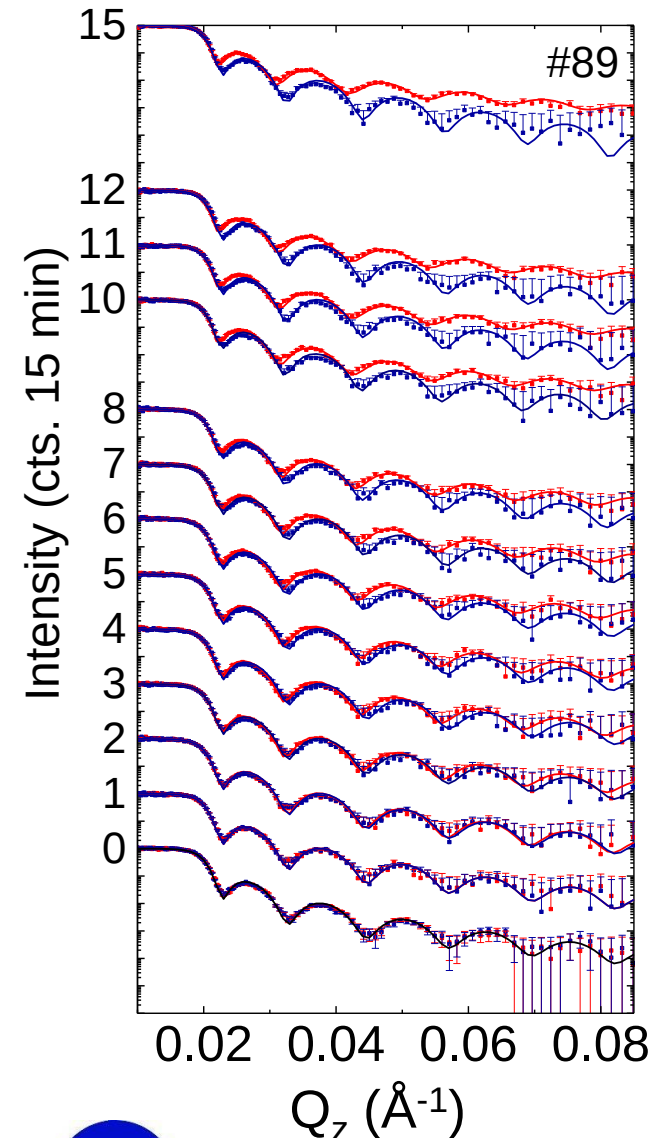


Results: SELENE @ AMOR

Cu on Si(100)



Modern Optics + *in-situ* Coating Facility



Prospects with ESS (→ 2019)



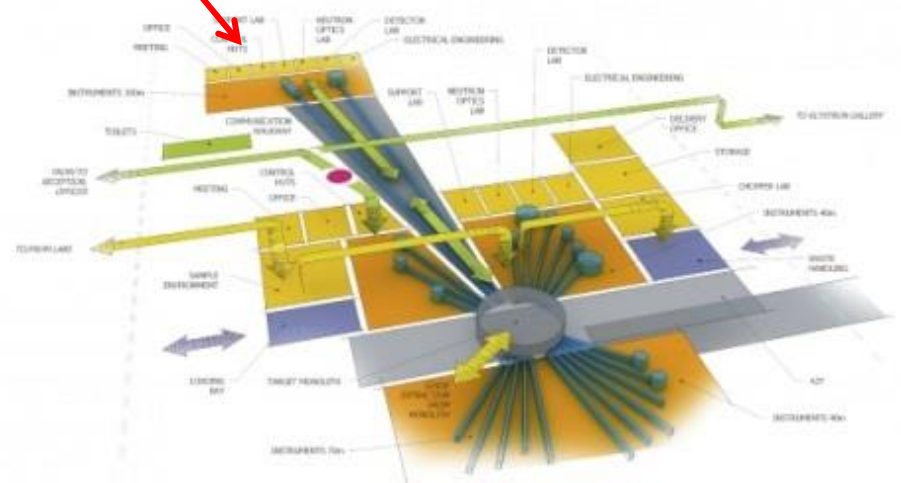
Book keeping:

- gain in brilliance: > 100
 - longer mirrors:
 - incr. of illum. area: > 10
 - divergence: > 4
 - free of charge: extended Q -range
- **gain factor > 4000**

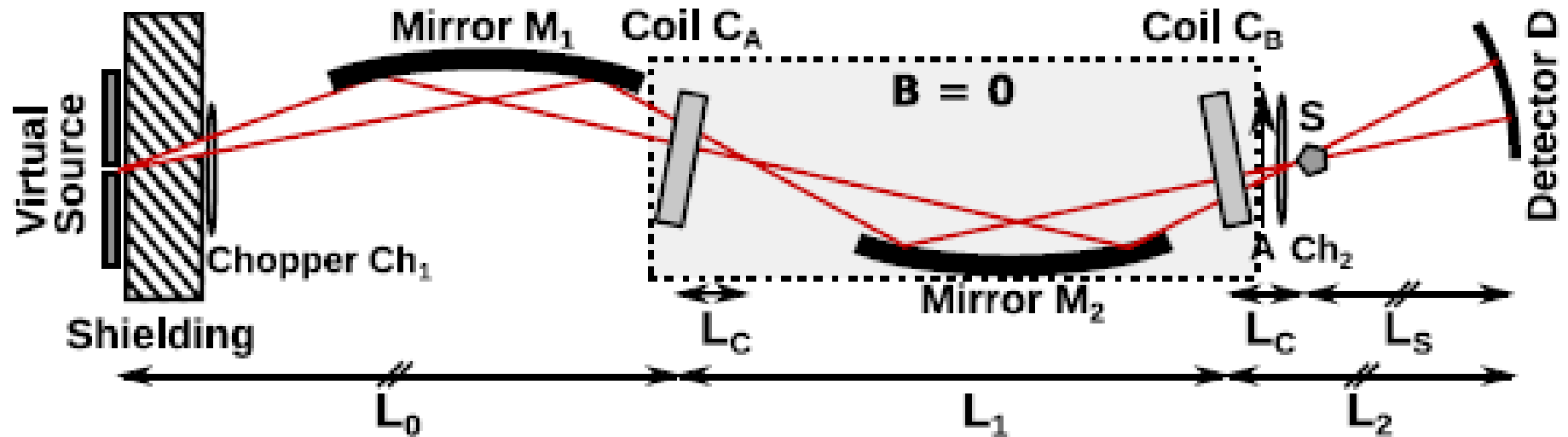
gain in measurement time:

- SELENE @ PSI:
 $T \cong 1$ hour/scan
- ESTIA @ ESS:
 $T < 1$ second

→ *in-situ* measurements
in real time



Other Implementations of Montel Optics: MIEZE



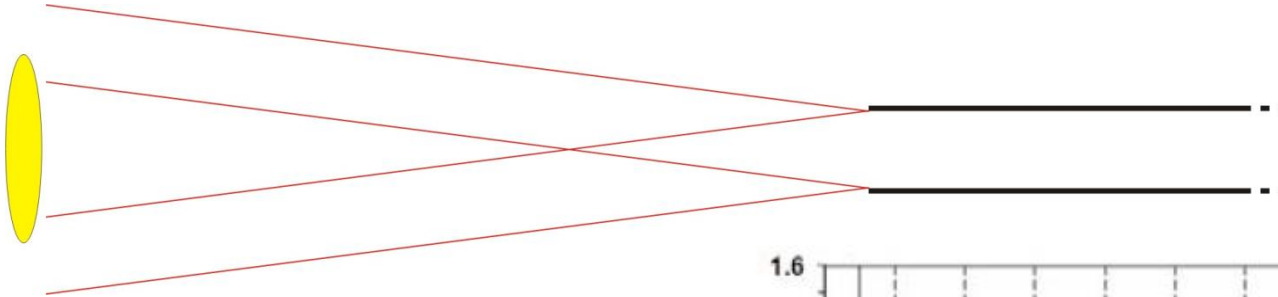
Possibly too advanced to be accepted by community
→ chance for existing facilities

Content

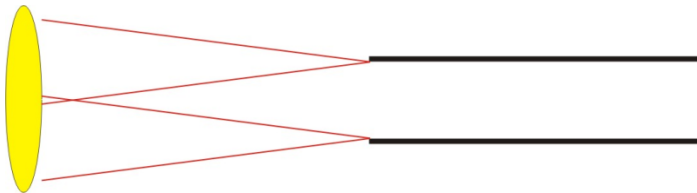
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Illumination Losses

under illumination $\rightarrow$ loss of intensity, moderator too small

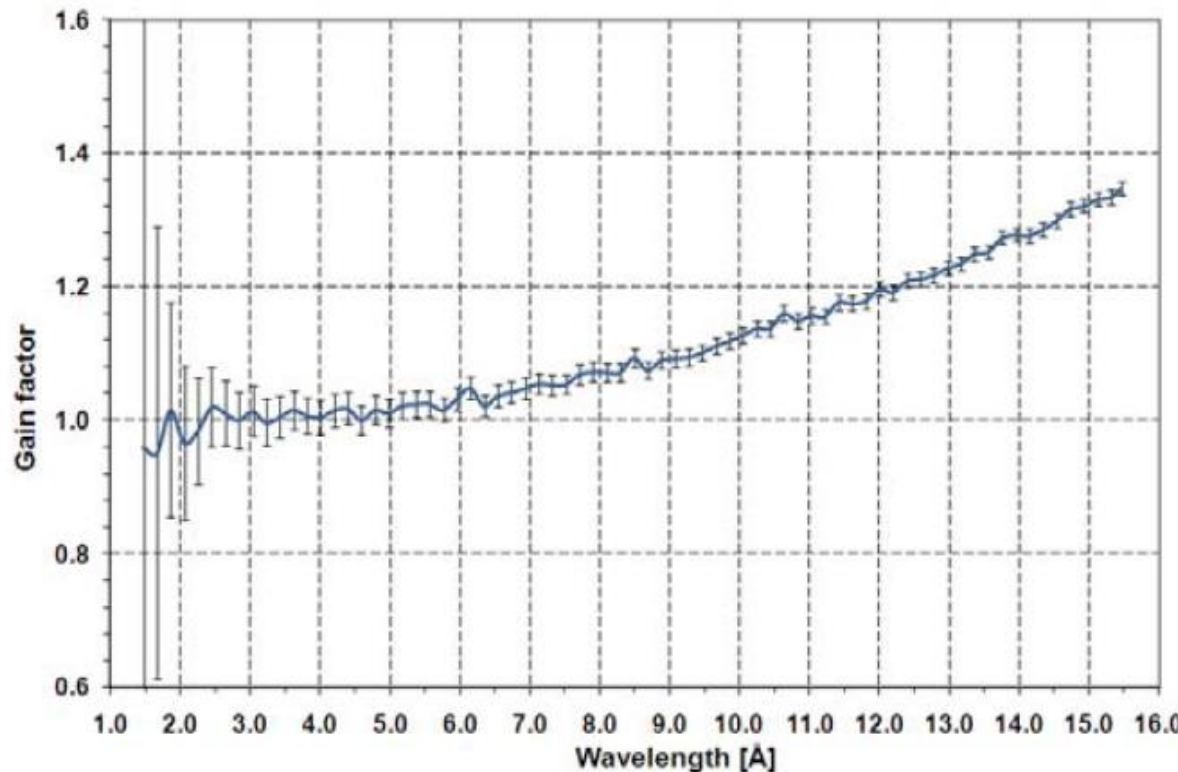


go close to moderator



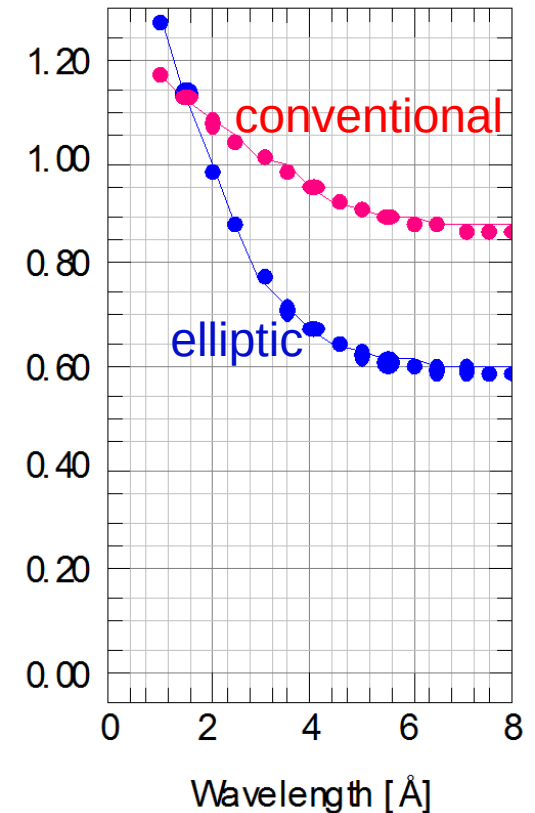
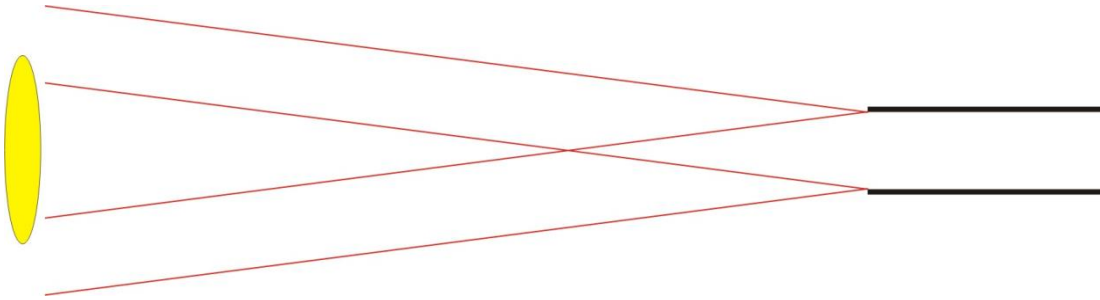
Example: NL1 @ FRM II

- 30% gain (2 m $\rightarrow$ 0.1 m)

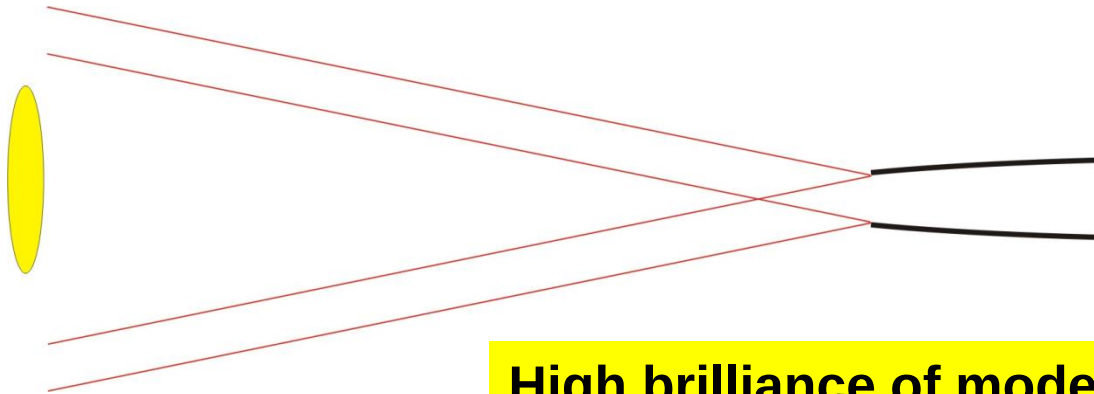


Small Source (example: Pancake Moderator @ ESS)

Straight guide: under-illumination



Elliptic/parabolic guides: even worse!

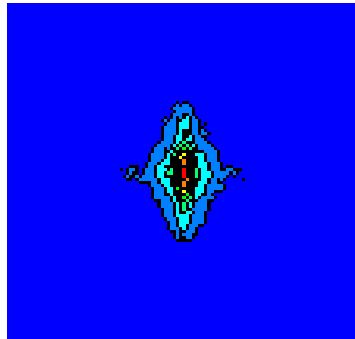
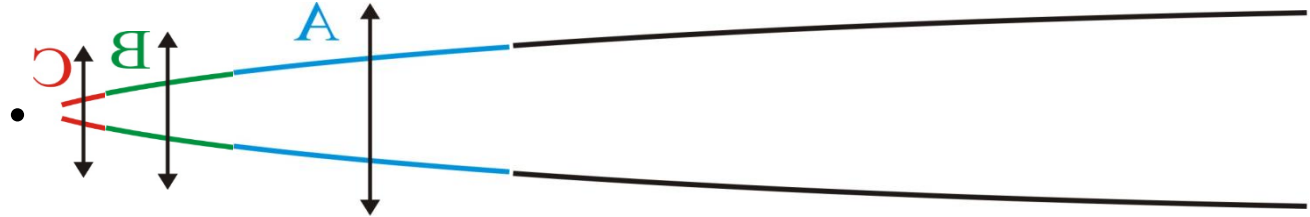


High brilliance of moderator is useful, if:

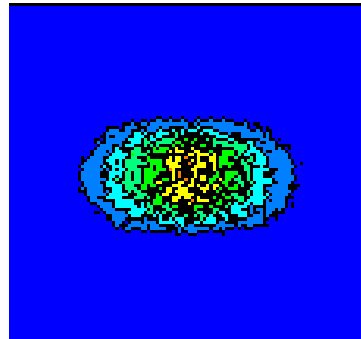
- guide is extended close to moderator
- **this condition may not be fulfilled at ESS**

Alternative Solutions

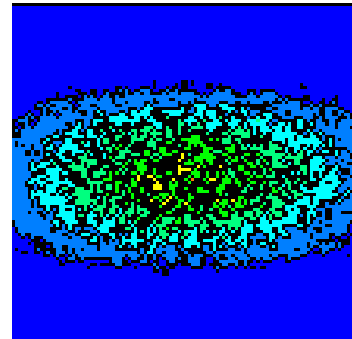
Guides:



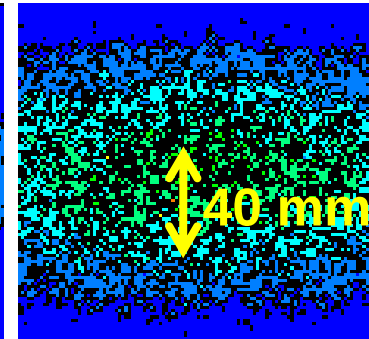
$f_{out} = 0.1 \text{ m}$



$f_{out} = 0.2 \text{ m}$

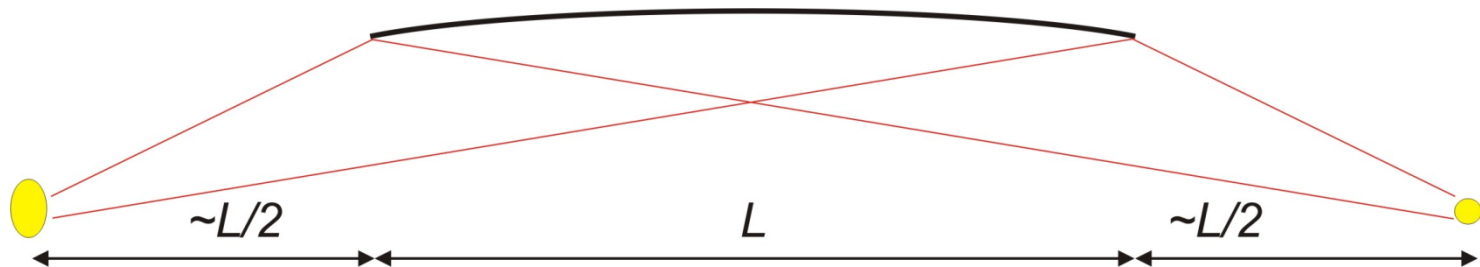


$f_{out} = 0.5 \text{ m}$



$f_{out} = 1.2 \text{ m}$

Montel Mirrors:



Content

- Introduction
- Supermirrors
- Transport
- Focusing Optics
- Montel Mirrors
- Beam Extraction
- Summary

Summary: Scientific Opportunities

- investigation of small samples facilitated:
 - novel materials
 - extreme conditions
 - quantum phase transition
- investigation of heterostructures
- in-situ / real time experiments

Summary: Technical

Flux considerations:

- maximum possible intensity (is anticipated experiment possible?)

$$I = \eta \cdot A \cdot \Delta\lambda \cdot \Omega \cdot \Psi$$

- consider Liouville's theorem

$\eta \cong 1$: brilliance transfer
(efficiency of transport)

Existing sources:

- new opportunities in beam optics
- „local“ upgrades of instruments possible (cheap and effective)

New sources:

- move guide entrances close to moderator: **not realized so far**
- extract only useful neutrons

Do not Use Monte-Carlo, Use First Your Brain

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- etc. (did I forget somebody?)

