Neutron Instrumentation Part 2

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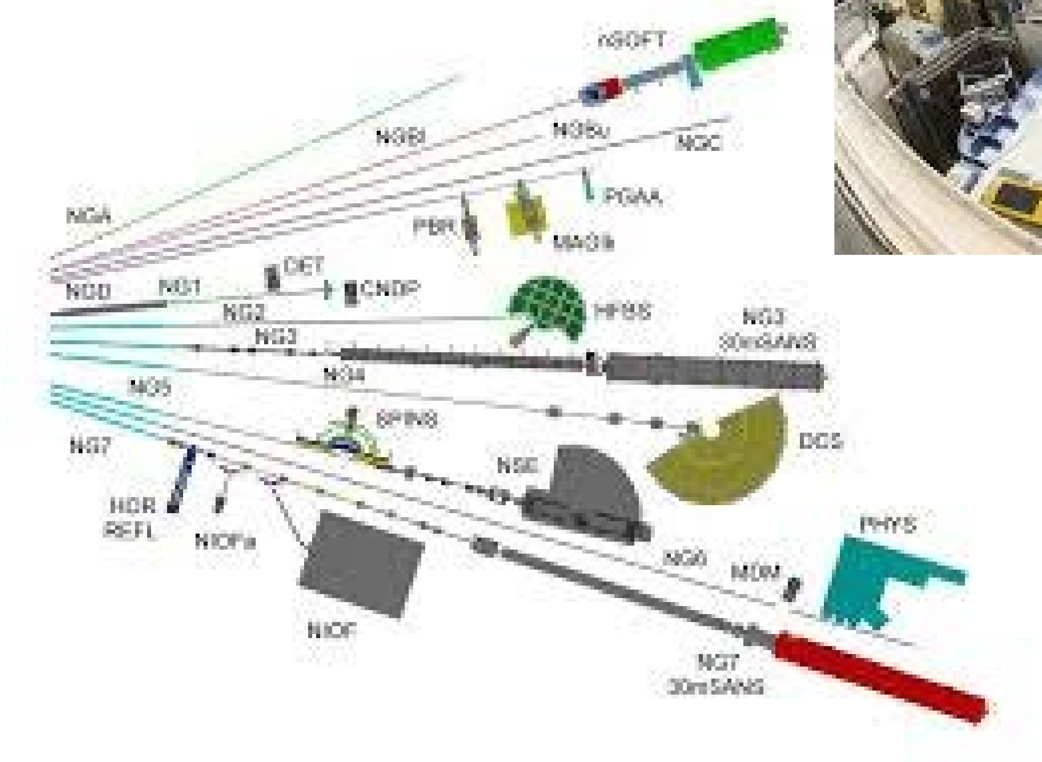
What we will cover in Part 2

- Why we need special optics
- Neutron reflection from surfaces (see Roger’s lecture)
- Reflecting Collimators
- Neutron Guides
- Some Aspects of focusing

What can you say about these pictures?



Need for specialized neutron optics

Problem

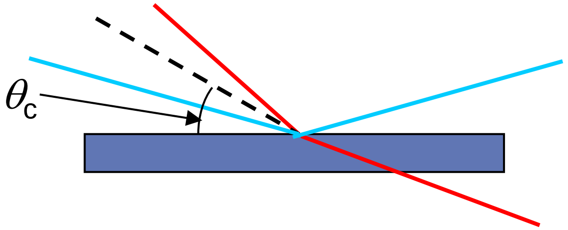
- Neutrons from the source go in all directions – most are not headed toward the sample.
- Number reaching the sample is proportional to the solid angle subtended by the sample at the source, which means it is proportional to $1/L^2$.
- Large instruments mean L is large, so not many neutrons reach the sample.

Another way of saying this, is that for many instruments natural collimation does not accept all the angular divergence that could be used in the experiment – angular resolution is too good!

Reflection/Refraction at Surfaces

Index of refraction

$$n = 1 - \lambda^2\rho/2\pi\ [-\ i\lambda\mu/4\pi]$$



λ = wavelength
ρ = Nb = scattering length density
μ = linear absorption length

n < 1 for most materials, so there is a critical angle θ_c for total **external** reflection

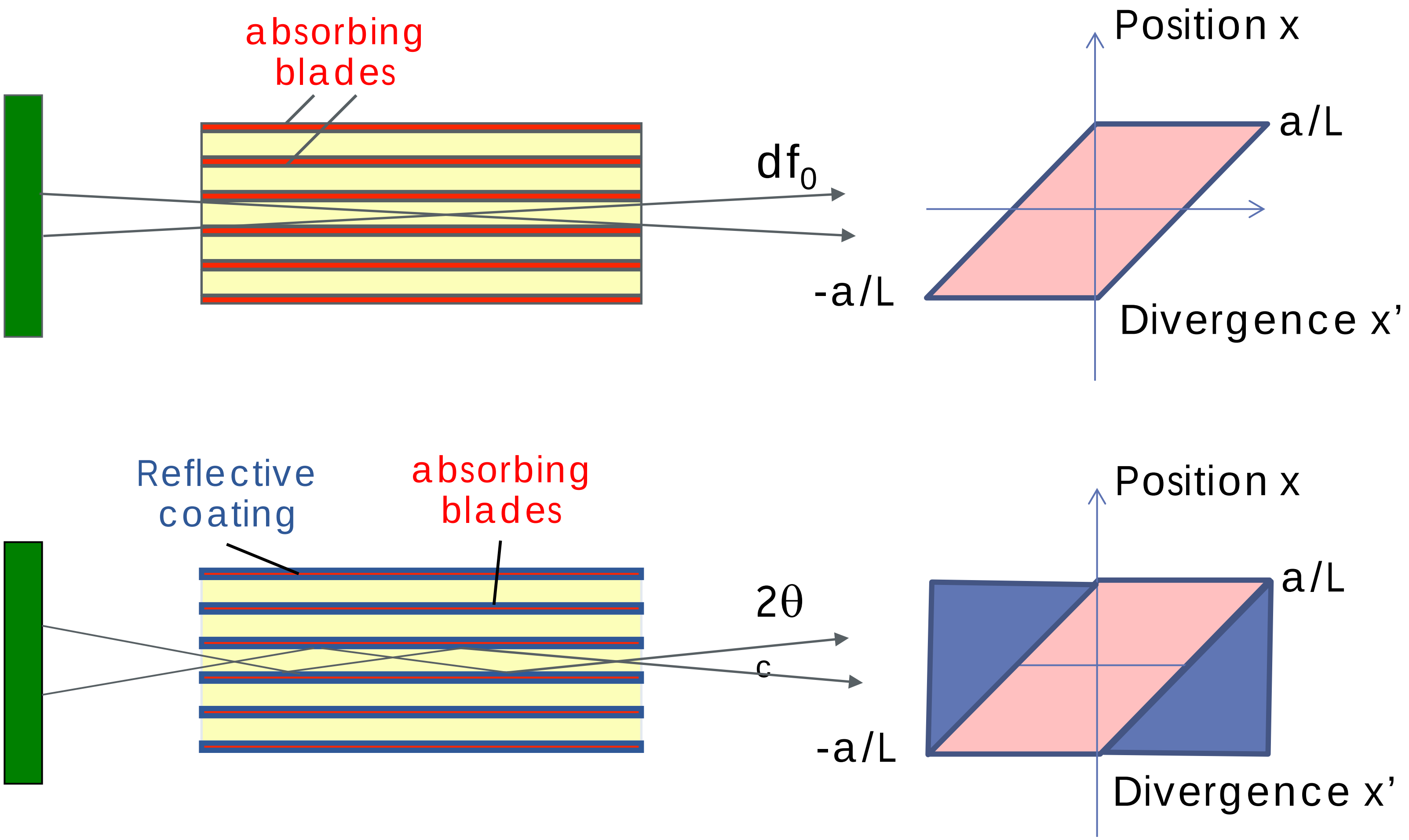
$$\theta_c = 1 - \lambda\sqrt{\rho/\pi} \longrightarrow$$

For Ni θ_c (°) = 0.1 λ (Å) θ_c (mrad) = 1.7 λ (Å)

	N ($\times 10^{29}/m^3$)	b ($\times 10^{-24}/m$)	Nb ($\times 10^{38}/m^2$)	θc (mrad)*)
^{58}Ni	9.0	1.44	1.0	2.03
Beryllium	12.3	0.77	9.5	1.73
Nickel	9.0	1.03	9.3	1.70
Iron	8.5	0.96	8.2	1.62
Carbon	11.1	0.66	7.3	1.61
Copper	8.5	0.79	6.7	1.39
Cobalt	8.9	0.25	2.2	0.86
Aluminium	6.1	0.35	2.1	0.81

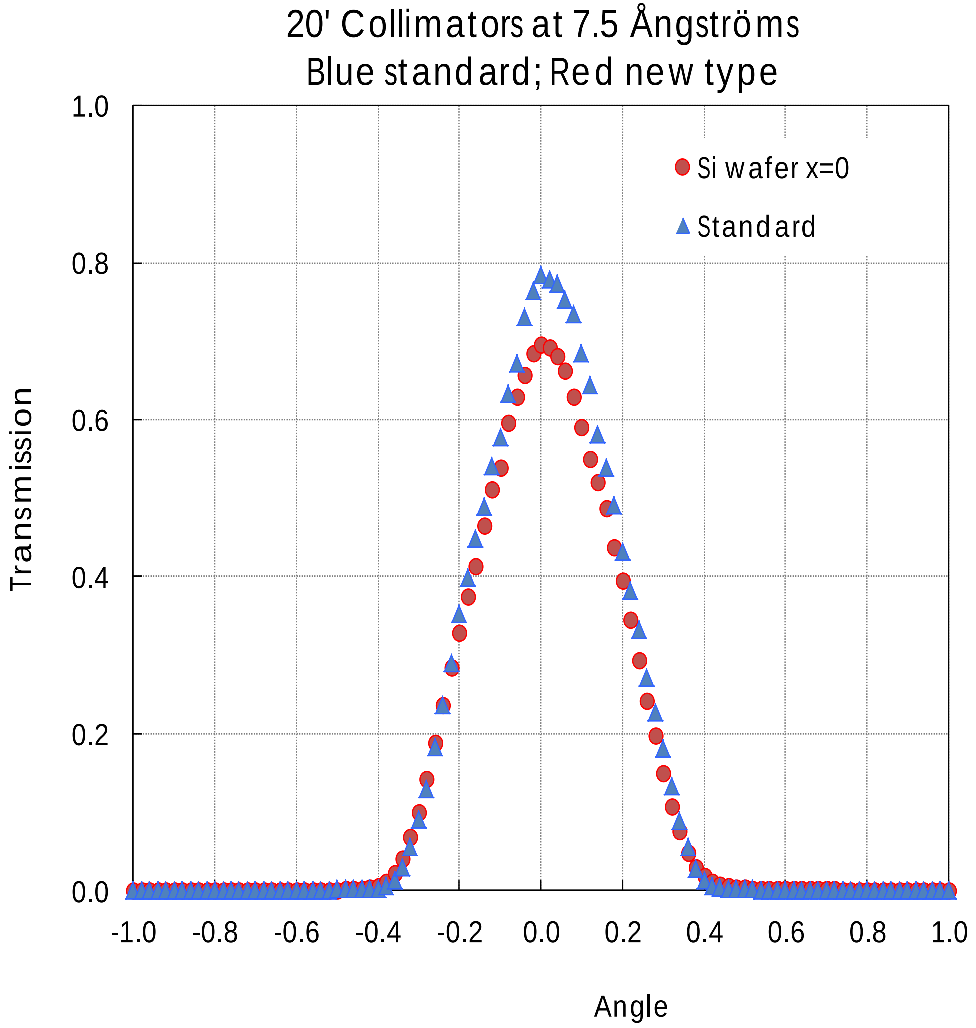
*1 mrad = 3.44 minutes of arc

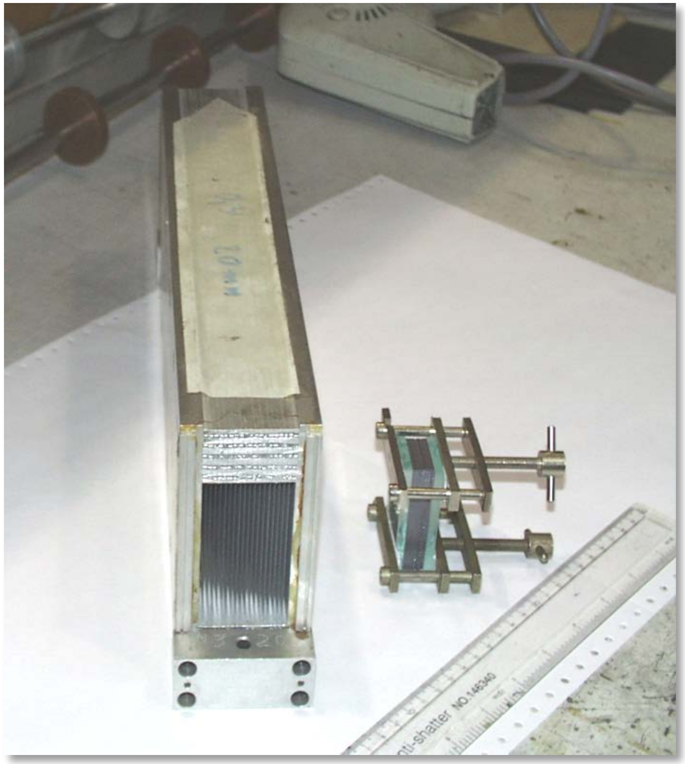
Reflecting collimators



Double the intensity, for same divergence, if $\theta_c = a/L$
Wavelength dependent

Reflecting collimators





Transmission over long distances – neutron guides

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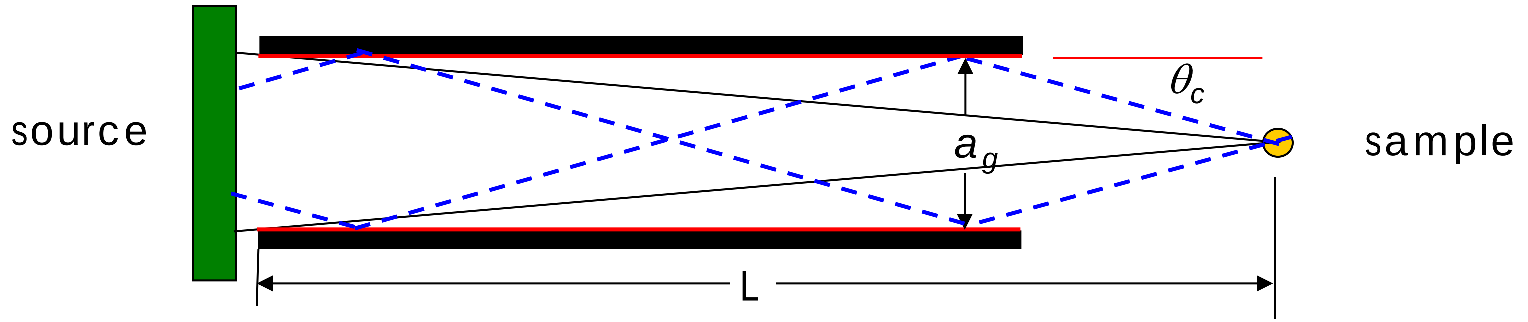
Neutron guides

Guides can increase the neutron flux at the sample by bringing more "divergence" to the sample. (Divergence is the range of incident angles measured relative to the nominal beam incident direction.)



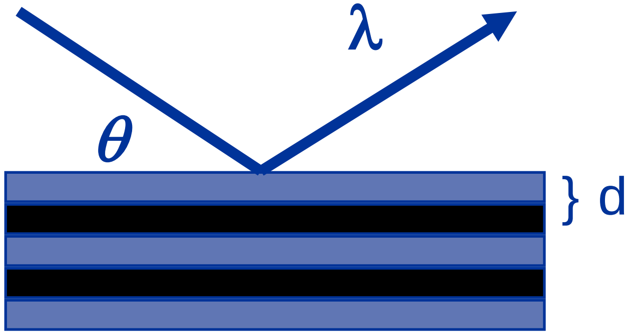
The effective "guide gain" is the flux reaching the sample with the guide compared to the flux reaching the sample with natural collimation.

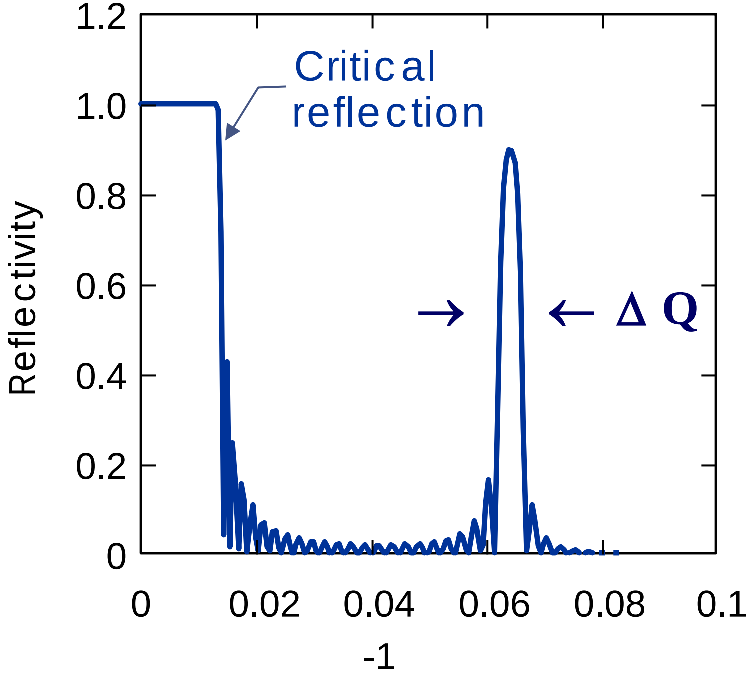
For an ideal **fully illuminated** and optimized straight guide this gain is

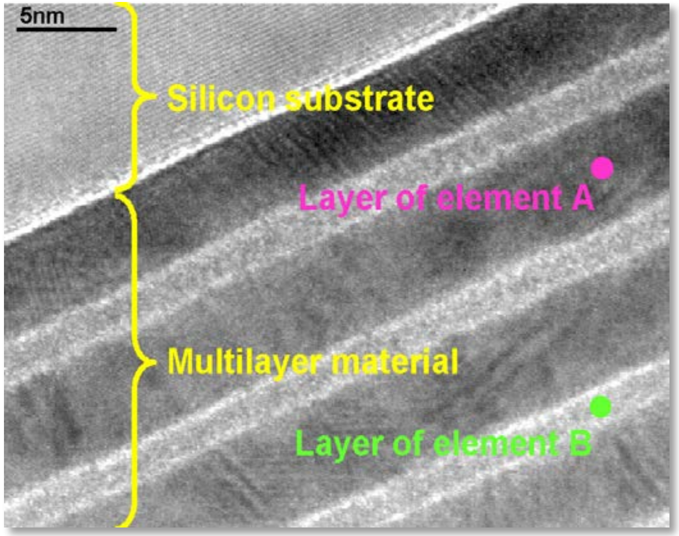
$$G_v = \frac{2\theta_c}{a_{gv}/L} \qquad G_h = \frac{2\theta_c}{a_{gh}/L} \qquad G = G_v G_h = \frac{4\theta_c^2 L^2}{a_{gv} a_{gh}}$$

For a Ni guide with $a_g = a_h = 10$ cm and L = 40, the guide gain at 6 Å is $G \sim 66$

Reflection from multilayers





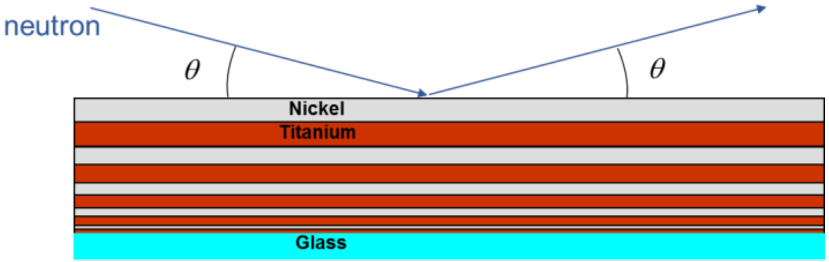


$$\theta \sim \lambda/2d$$

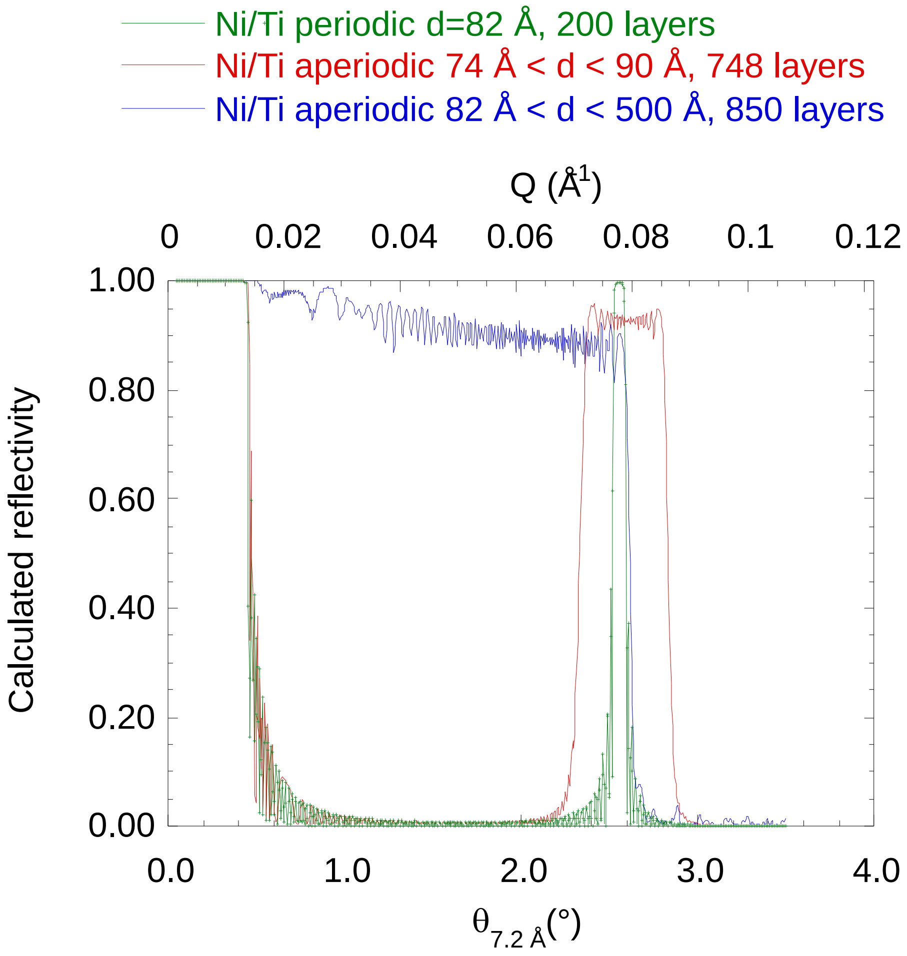
$$R = \frac{4N^2 d^4 (Nb_1 - Nb_2)^2}{\pi^2 n^4}$$

$$\frac{\Delta\lambda}{\lambda} = \frac{2d^2 (Nb_1 - Nb_2)}{\pi}$$

An introduction to supermirrors



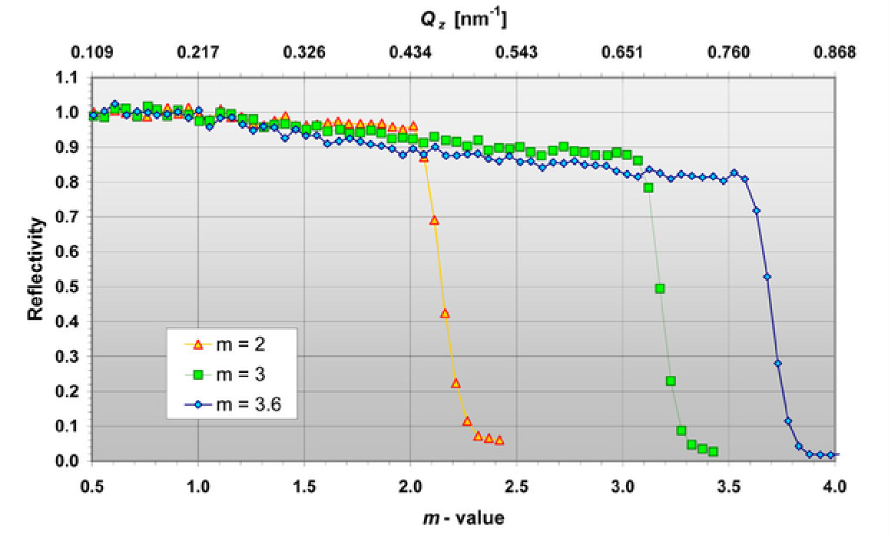
Material	Nb (x10^{-38} m^{-2})
^{58}Ni	13.31
Diamond	11.71
Ni	9.41
Quartz	3.64
Germanium	3.64
Silver	3.50
Aluminium	2.08
Silicon	2.08
Vanadium	-0.27
Titanium	-1.95
Manganese	-2.95

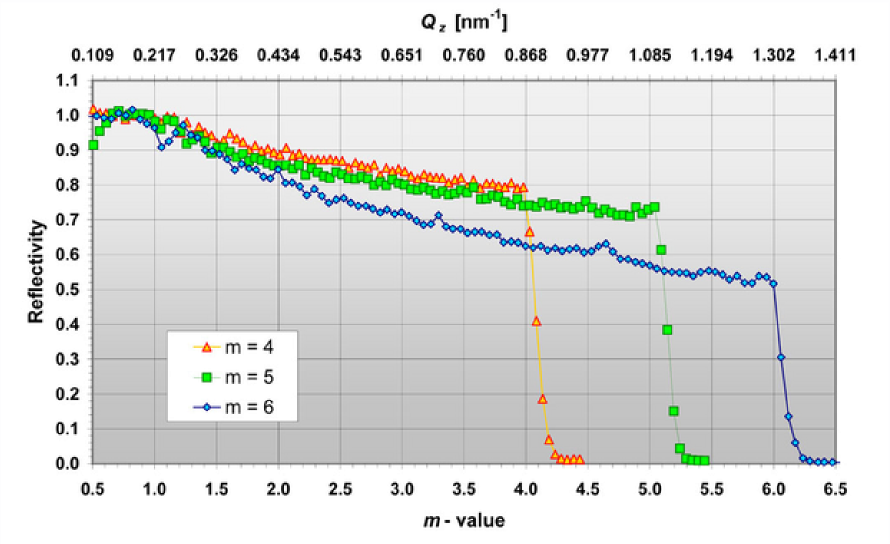


Supermirror guides

Modern Supermirror capabilities (NiTi)

“Effective critical edge” is *m* times the critical edge of natural Nickel





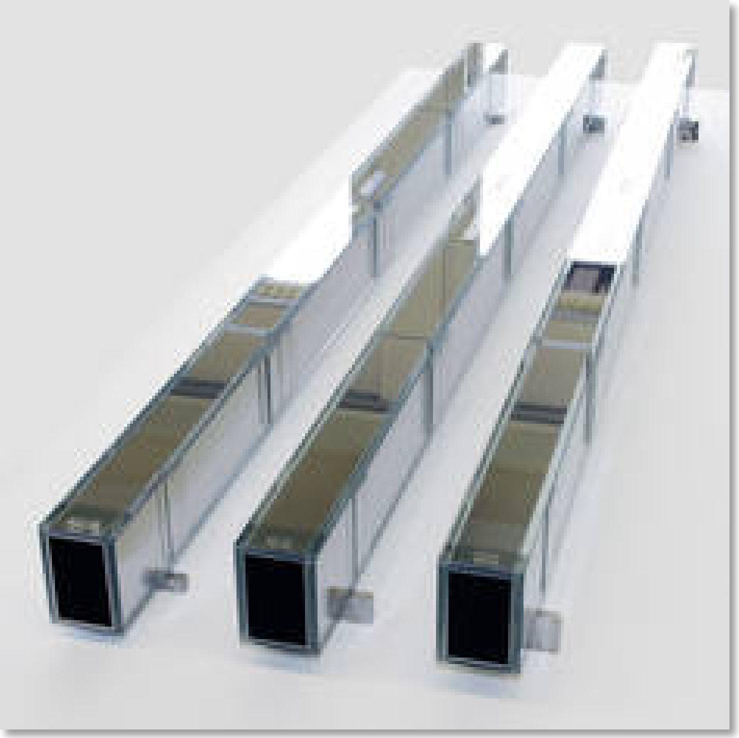
Swiss Neutronics
http://www.swissneutronics.com/products/coatings.html

$$m = \frac{\theta_c^{eff}}{\theta_c^{Ni}}$$

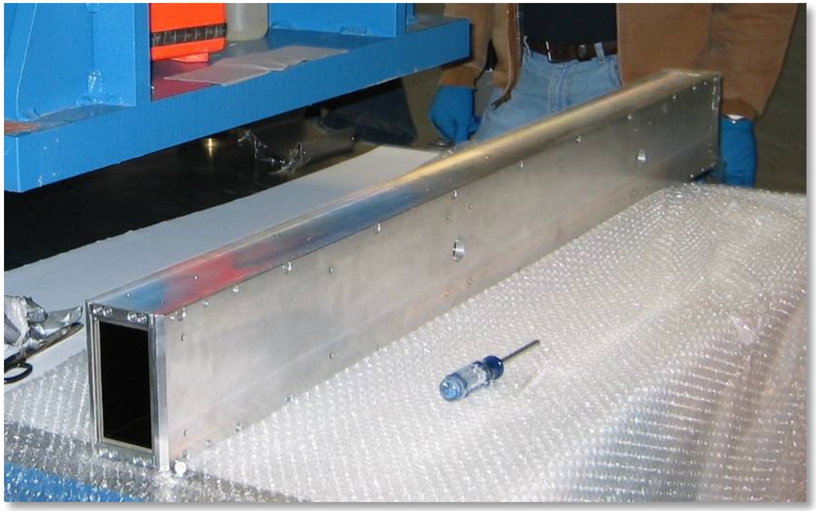
$$G = \frac{4m^2\theta_{Ni}^2 L^2}{a_{gv}a_{gh}}$$

But be careful the reflectivity!
For a neutron travelling at 4 θ_c^{Ni} in a 100m long guide of 5 cm width:
Number of reflections, n ~ 14,
Transmission = R^n = 4% !!

Typical neutron guides

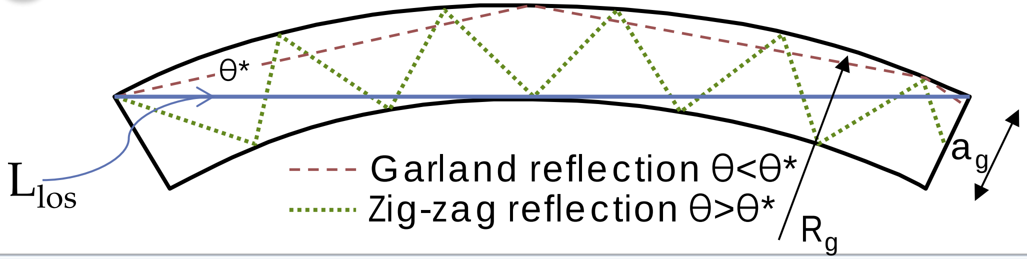


- Segments of a long guide
- Each segment is made up of several ~1/2 m sections joined together
- Glass is sufficiently thick to support the guide vacuum



Segment of guide in a steel vacuum housing

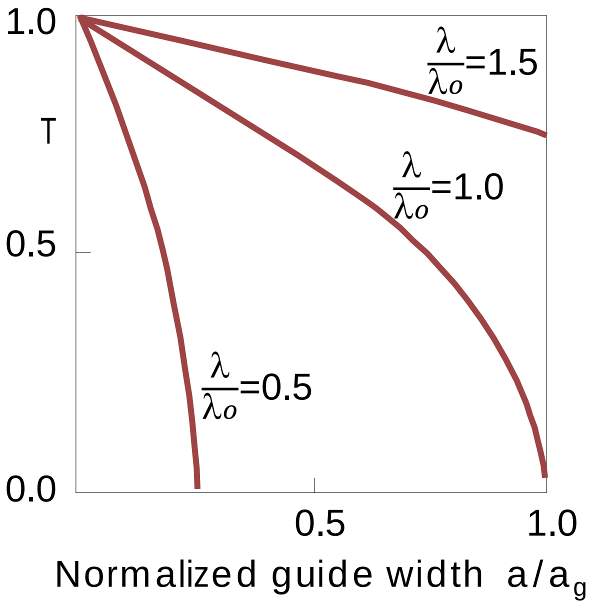
Curved guides can eliminate fast neutrons



Neutrons must make at least one reflection to get through the guide. Fast neutrons have extremely small critical angles for reflection, and so are unlikely to be transmitted.

Line-of-sight length L_{los} is related to the guide radius of curvature R_g and the guide width a_g

$$L_{los} \approx (8\ a_g\ R_g)^{1/2}$$



Characteristic wavelength

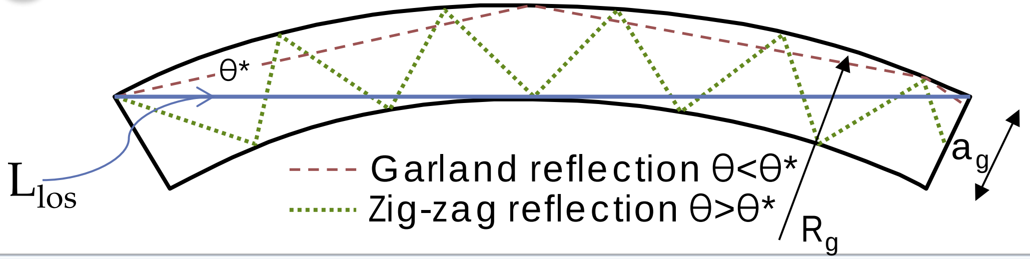
$$\lambda_0 = (1/m)(\pi/\rho)^{1/2}(2a_g/R_g)^{1/2}$$

$$= (573/m)\ (2a_g/R_g)^{1/2} \quad \text{for } \lambda_0 \text{ in Å.}$$

(ρ = scattering length density = Nb_{coh})

Neutrons with $\lambda < \lambda_0$ can only reflect from the outer guide surface ("garland reflections").

Curved guides can eliminate fast neutrons



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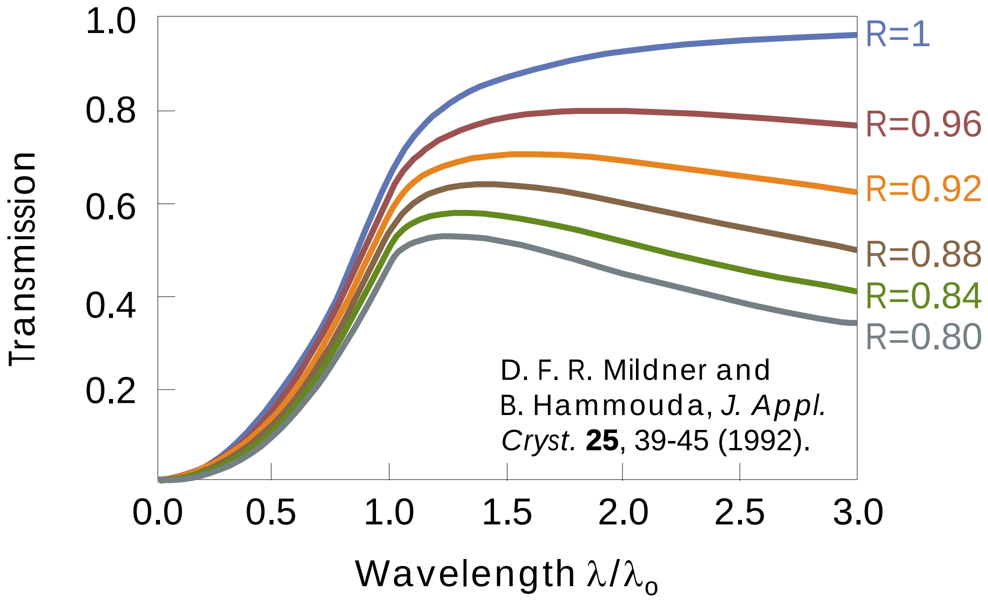


D. F. R. Mildner and B. Hammouda, *J. Appl. Cryst.* **25**, 39-45 (1992).

Characteristic wavelength

$\lambda_0 = (1/m)(\pi/\rho)^{1/2}\,(2a_g/R_g)^{1/2}$

$= (573/m)\ (2a_g/R_g)^{1/2}$ for λ_0 in Å.

(ρ = scattering length density = Nb_{coh})

Neutrons with $\lambda < \lambda_0$ can only reflect from the outer guide surface ("garland reflections").

An Example of a curved guide at SNS

Curved part of the ~82 m long guide at the SNS backscattering spectrometer. The guide is in the black steel vacuum housing. It rests on rigid steel support beams that are not visible in the picture.

a_g = 10 cm internal, 11 cm external

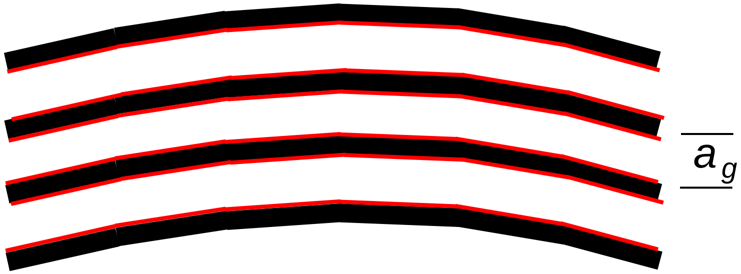
R_g = 1000 m

$L_{los} \approx 30$ m

$m = 2.5$

$\lambda_0 \approx 3.2$ Å

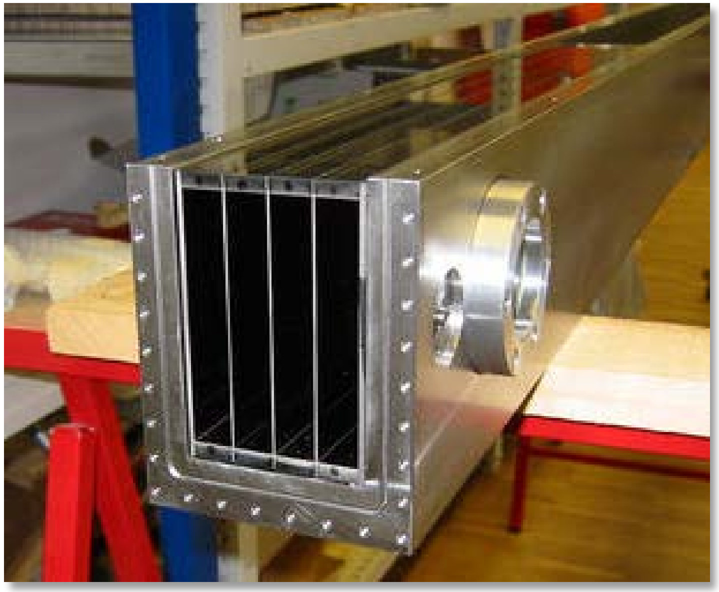
Neutron multi-channel guide ("beam bender")



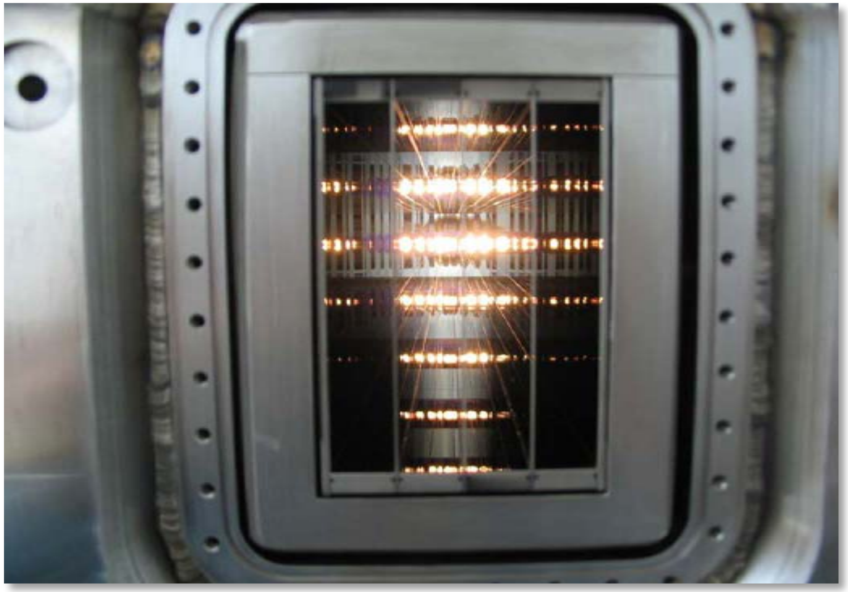
Characteristic wavelength

$\lambda_0 = (1/m)(\pi/\rho)^{1/2}(2a_g/R_g)^{1/2}$

Making a_g smaller allows R_g to be smaller for the same characteristic wavelength, so the beam can be bent more sharply



SNS BL4 bender being assembled



BL4 bender installed in shutter insert

Example

Assume we would like to bring out a 5 cm wide guided beam of $\lambda \geq 2$ Å neutrons, and need to get out of the line of sight over a guide distance of 8 m.

$$\boxed{\mathrm{L}_{\mathrm{los}} = (8\, a_g\, R_g)^{1/2} \quad \rightarrow \quad R_g = 160\ \mathrm{m}}$$

$$\lambda_0 = (573/m)\,(2a_g/R_g)^{1/2} \quad \rightarrow \quad \lambda_0 = 14.3\ \text{Å} \quad \text{for} \quad m = 1$$

A simple curved guide will not produce the desired results !!!

$$\boxed{\text{Try 7 channels with } m = 1.\ \text{ This gives } a_g = 0.71\ \text{cm.}}$$

$$L_{los} = (8\, a_g\, R_g)^{1/2} \quad \rightarrow \quad R_g = 1127\ \mathrm{m}$$

$$\lambda_0 = (573/m)\,(2a_g/R_g)^{1/2} \quad \rightarrow \quad \lambda_0 = 2.0\ \text{Å} \quad \text{for} \quad m = 1$$

This combination produces the desired results !!!

Some aspects
of guide performance

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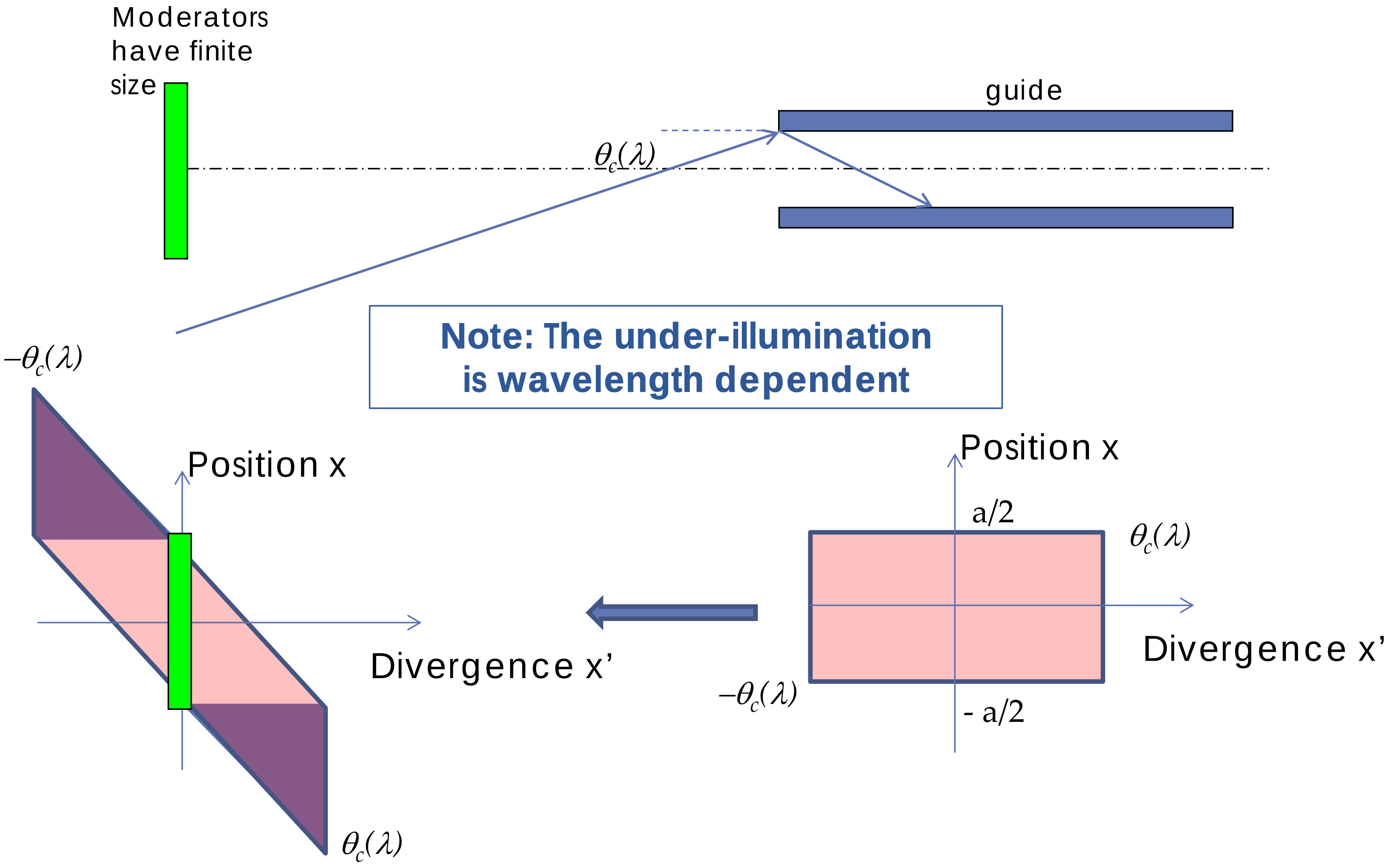
Neutron guide specification

Neutron guides are typically made by depositing the coating (usually Ni or supermirror) on smooth glass substrates. After coating, these substrates are joined together and aligned to make up the desired guide profile.

Some things to think about when you are considering performance:

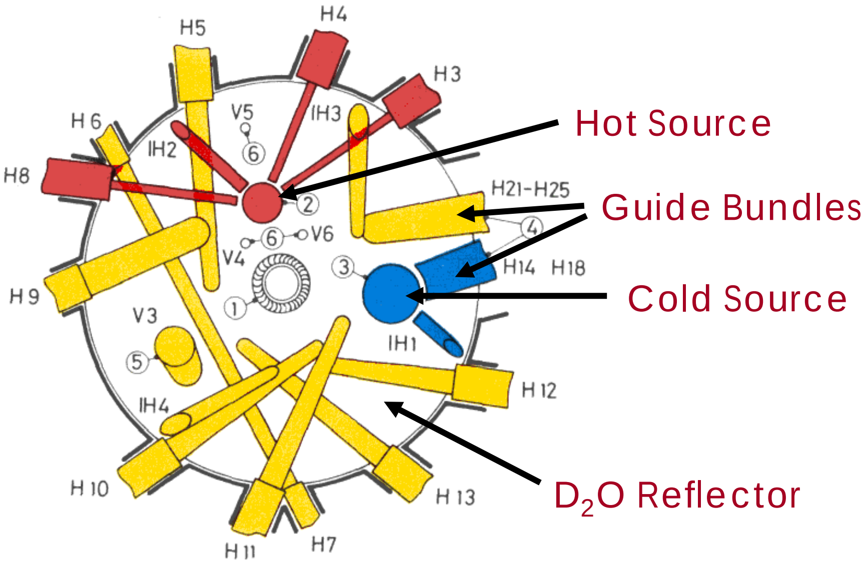
- Illumination
- Deviations from the desired profile result in a degradation of performance:
  - Surface roughness or waviness
  - Imperfections in coating
  - Gaps in guide
  - Steps at joints
  - Angular misalignment

Guide illumination



Note: The under-illumination is wavelength dependent

Guide bundle at a reactor



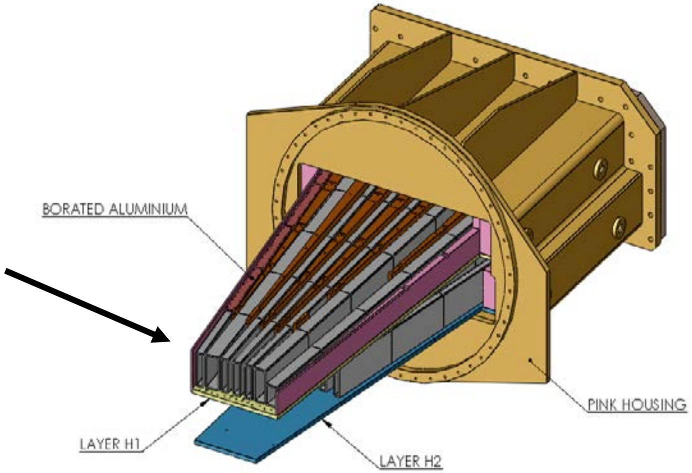
Hot Source

Guide Bundles

Cold Source

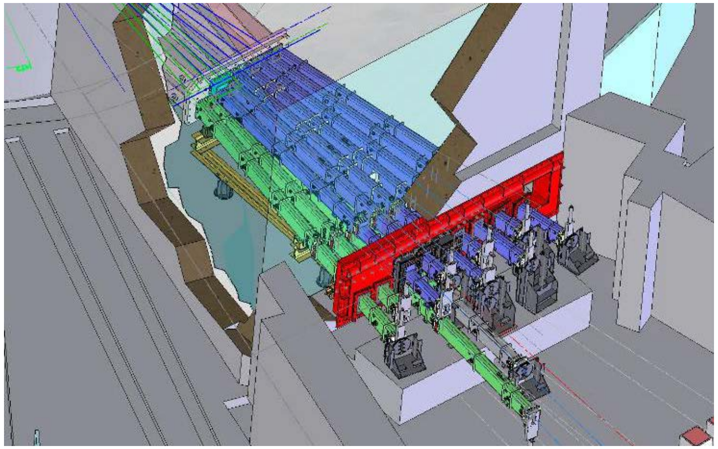
D_2O Reflector

ILL beam tubes – from ILL “Yellow Book”



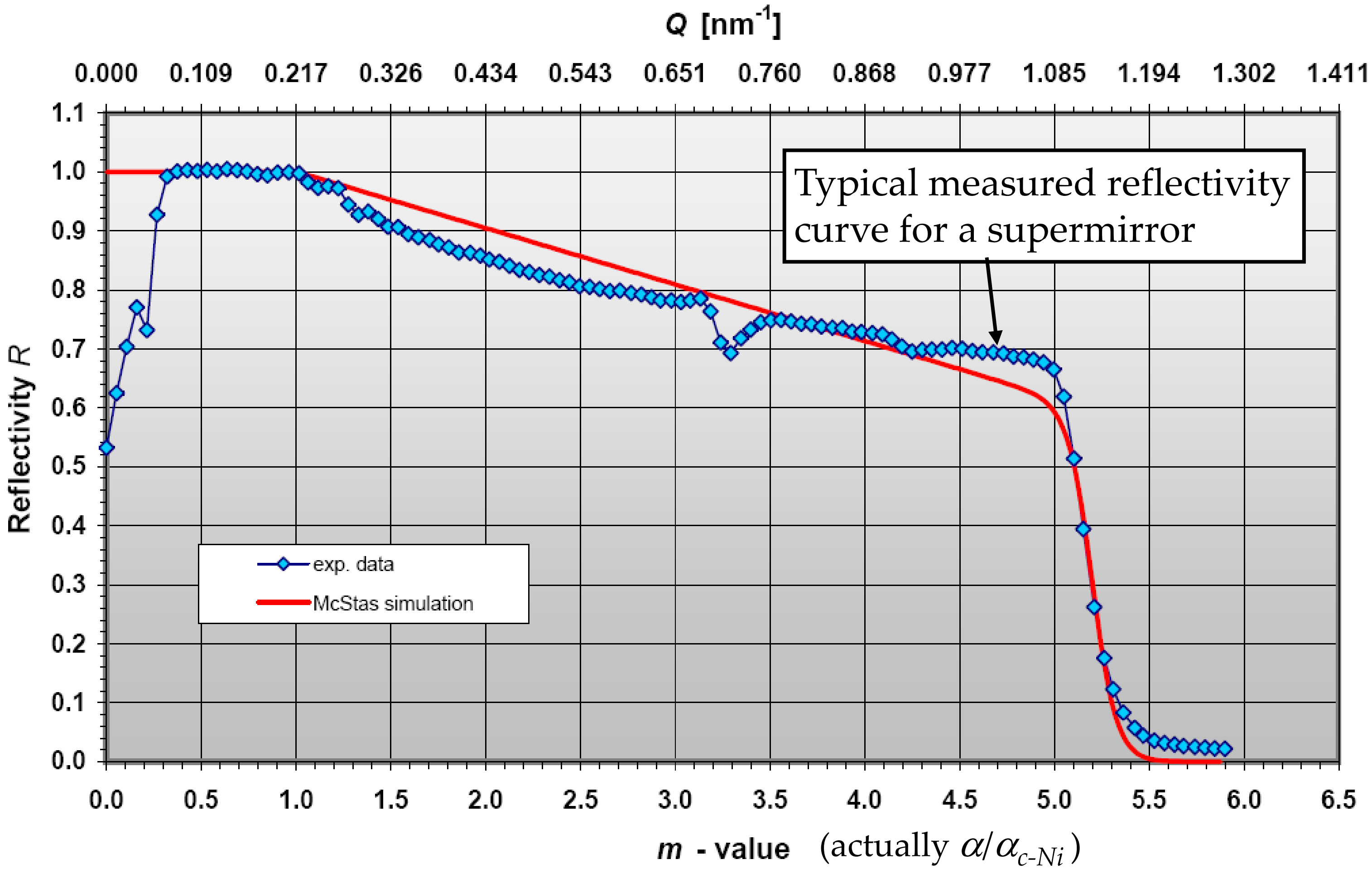
In pile section of guides supplying the big guide hall at ILL. The 7 cold guides of the top layer focus on the vertical cold source, the 5 thermal guides of the bottom layer focus on the thermal beam nose.

K. H. Anderson, et al.,
“The neutron guide system of ILL”,
in *Proceedings of the International Symposium on Research Reactor and Neutron Science*
- In Commemoration of the 10th Anniversary of HANARO,
Daejeon, Korea, April 2005



Swimming pool section of the 7 cold and 5 thermal guides.

Coating imperfections



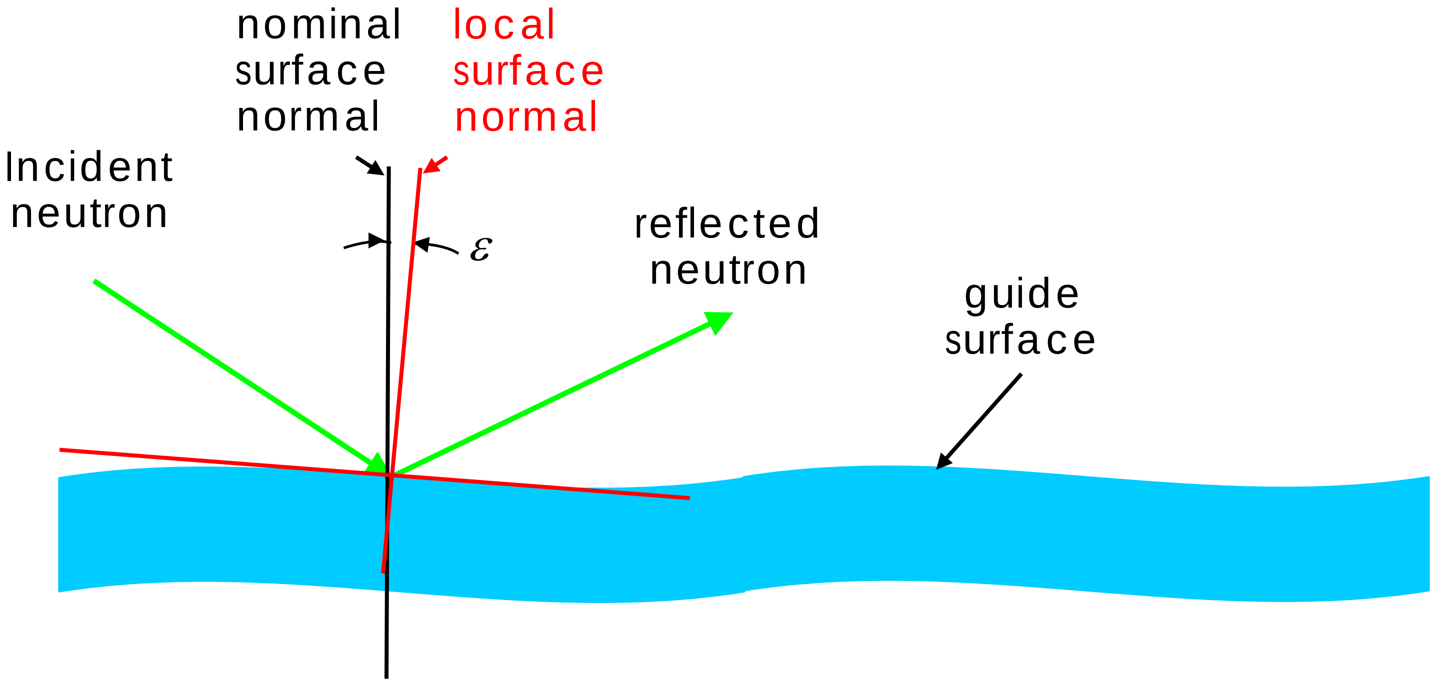
Typical measured reflectivity curve for a supermirror

Supermirrors have reflectivities significantly less than 1.

Probability of transmission is low if multiple reflections are required.

Surface roughness or waviness

Waviness: Length scale for variations >> neutron wavelength



Guide surface appears to be flat locally, so reflection is specular but with different angle. This is roughly the same as having many short guide sections with slight misalignments between each section. The effects should be small if the distribution of ε is narrow compared to the critical angle. Quantitative assessment is possible with Monte Carlo simulation.

Surface roughness or waviness (continued)

Roughness: Length scale for variations ≈ neutron wavelength

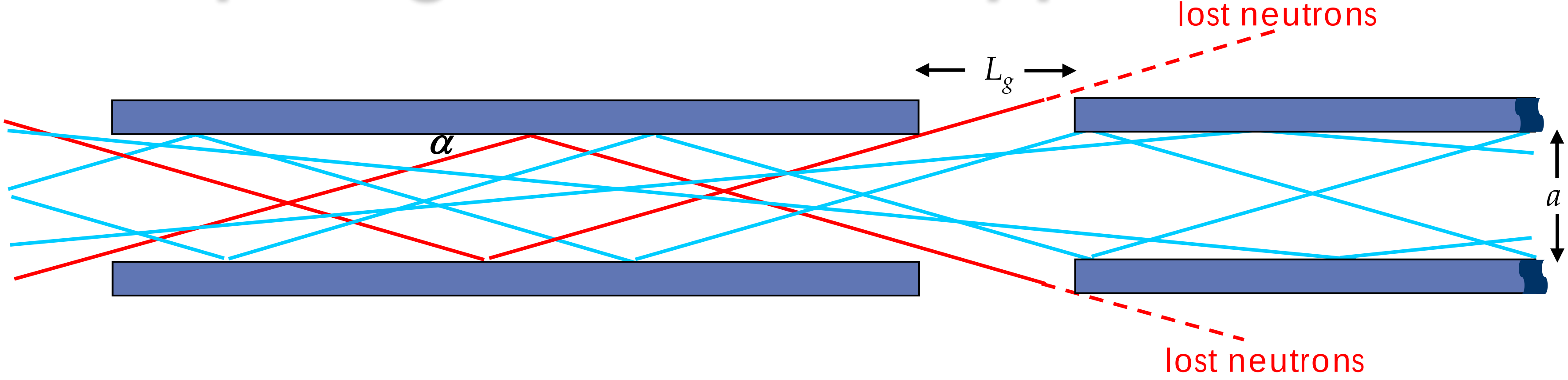
Roughness on microscopic and mesoscopic scales leads to diffuse scattering (*i.e.* neutrons scattered at angles other than the incident angle) in addition to the specular scattering. This becomes a diffraction problem and cannot be represented by the classical ray-tracing methods discussed so far. From a practical perspective, the reflecting surface of a guide or other optic needs to be as microscopically and mesoscopically smooth as is practical. Roughness in the range of a few Å is practical with polished glass substrates.

For further discussion of scattering from rough surfaces, see:

Sinha, S. K., Sirota, E. B., Garroff, S., and Stanley, H. B. (1988). *X-ray and neutron scattering from rough surfaces.* Phys. Rev. B **38**, 2297-2311.

Pynn, R (1992). *Neutron scattering by rough surfaces at grazing incidence.* Phys. Rev. B. **45**, 602-612.

Gaps in guide – crude approximation!



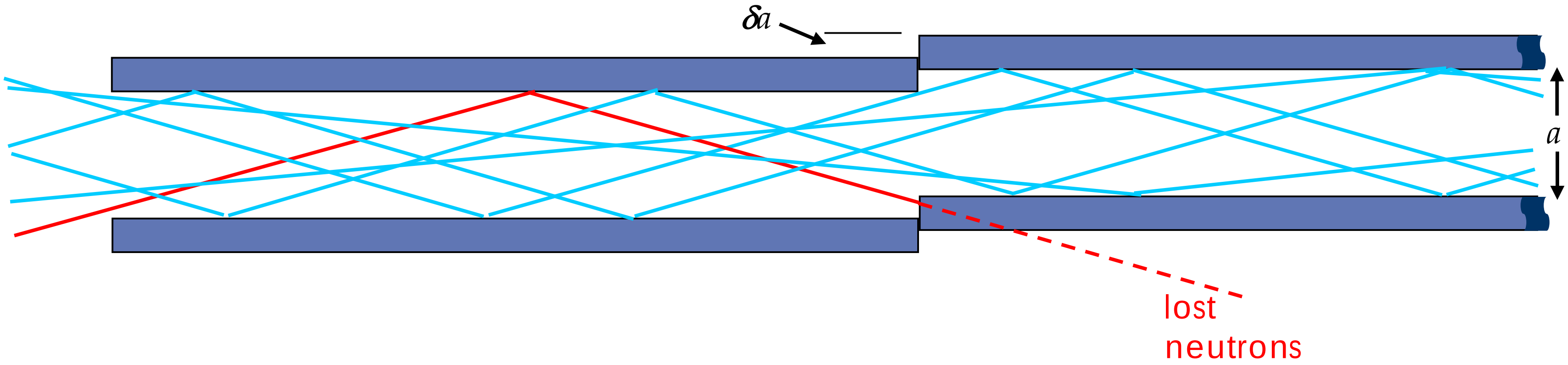
The probability of loss in the gap for a neutron at angle α relative to the guide axis is roughly the ratio of the gap length to the distance the neutron travels between reflections.

Probability of loss in one dimension $\approx L_g / (a / \alpha)$

This must be added to the probability of loss in the other dimension (width b)

Total probability of loss in gap $\approx L_g / (a / \alpha) + L_g / (b / \alpha)$

Steps at joints – crude approximation!



The main source of loss at the joint is neutrons striking the edge of the following guide section. For a filled guide, the fraction of neutrons striking the edge is roughly the fraction of the guide area covered up by the ends of the following section.

Probability of loss in one dimension ≈ $\delta a / a$

This must be added to the probability of loss in the other dimension (width *b*)

Total probability of loss at a single joint ≈ $\delta a / a + \delta b / b$

Losses at subsequent joints are roughly cumulative!!!

Example

Consider 50m of guide made up of 0.5m sections, with $a = b = 5$ cm

Assume sections are aligned to within 0.002 inch (50 microns) at each joint

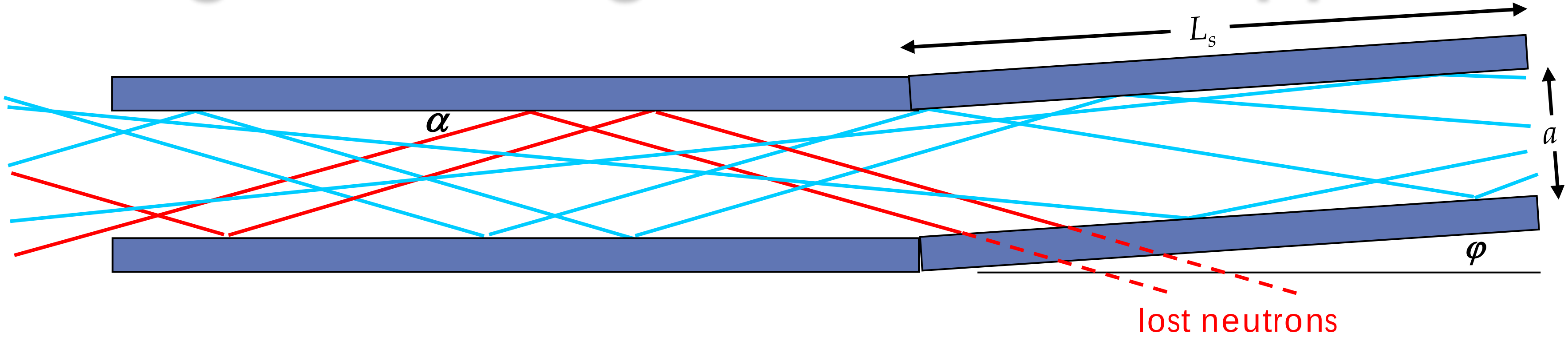
$$\delta a / a = \delta b / b = 0.001$$

$$\text{transmission} \approx (1 - \delta a / a - \delta b / b)^{100} = (0.998)^{100} = 0.82$$

Losses can be significant even for relatively good alignment!

Careful acceptance diagram or Monte Carlo treatment would show somewhat different results, because the treatment here is only approximate. However, the number calculated as above provides a quick estimate of the size of the effect and a check on the more precise calculation, and should represent a worst-case scenario.

Angular misalignment – crude approx.!



Neutrons that would have struck the lower surface of the tilted section at an angle α will now impact at a higher angle $(\alpha+\varphi)$. If $(\alpha+\varphi) > \alpha_c$, then the neutron will no longer be reflected and will be lost. In all other cases, all reflection angles at both surfaces of the tilted section will be shifted by the tilt angle φ, and this will propagate to subsequent sections.

Probability of loss $\approx 0.5 \times 0$ for $\alpha \le \alpha_c - \varphi$ and $a/\alpha \le L_s$

$\approx 0.5 \times 1$ for $\alpha > \alpha_c - \varphi$ and $a/\alpha \le L_s$

$\approx L_s\alpha/2a \times 0$ for $\alpha \le \alpha_c - \varphi$ and $a/\alpha > L_s$

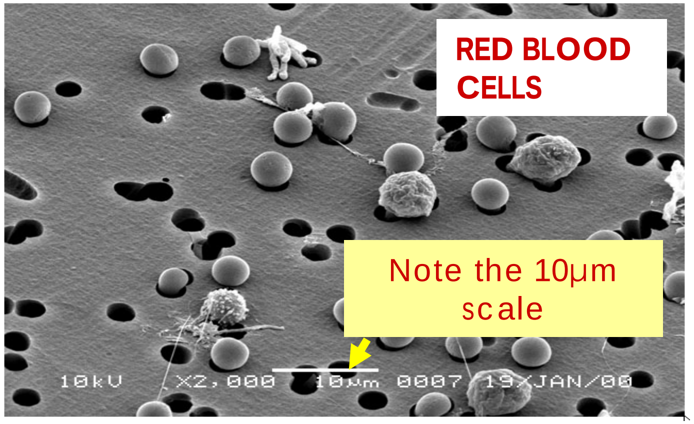
$\approx L_s\alpha/2a \times 1$ for $\alpha > \alpha_c - \varphi$ and $a/\alpha > L_s$

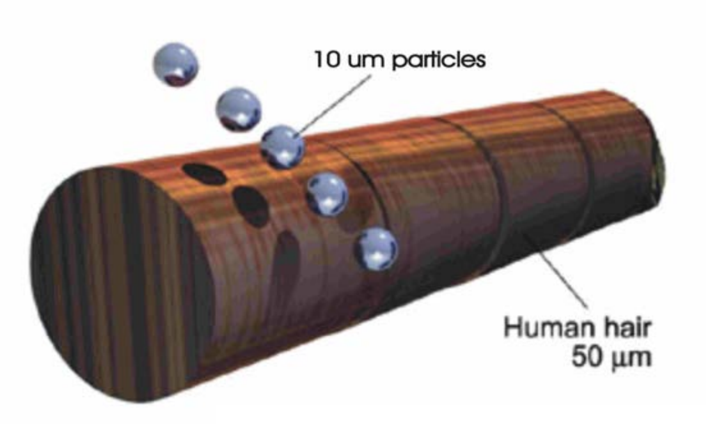
probability neutron will hit lower surface of misaligned section

probability neutron will not be reflected

Losses at subsequent misalignments are roughly cumulative!!!

What is practical?





Images provided by Joe Error

Alignment to better than 50 microns may be possible in a controlled laboratory environment, but is virtually impossible in a field application such as the installation of a neutron scattering instrument in a large experimental hall !

50 micron end-to-end misalignment for a 0.5m long guide segment

→ $\varphi = 0.0001$ radian

Since $\alpha_c = 0.0017\,\lambda$ radians (for λ in Å) is the critical angle of Ni

→ **Misalignment error is small but not negligible**

Monte Carlo simulations

- Monte Carlo methods simulate the performance of an instrument by tracing the paths of individual neutrons through the instrument. The neutrons are chosen randomly (with appropriate probabilities) from a phase-space ensemble representing the source (position and angle coordinates chosen to match the probabilities of those coordinates for this particular source).
- At each interface the neutron encounters (e.g., absorbing collimator surface, guide surface, neutron chopper, etc.) the outcome (absorption, reflection, etc.) is chosen from a probability distribution representing the physics of the neutron interaction at the interface.
- Typically, at least a few million neutron trajectories are calculated to give a good representation of the performance of the instrument.

Several different code packages are available to facilitate inputting the geometry and physics for the different beamline components. The most commonly used package is McStas

Focusing

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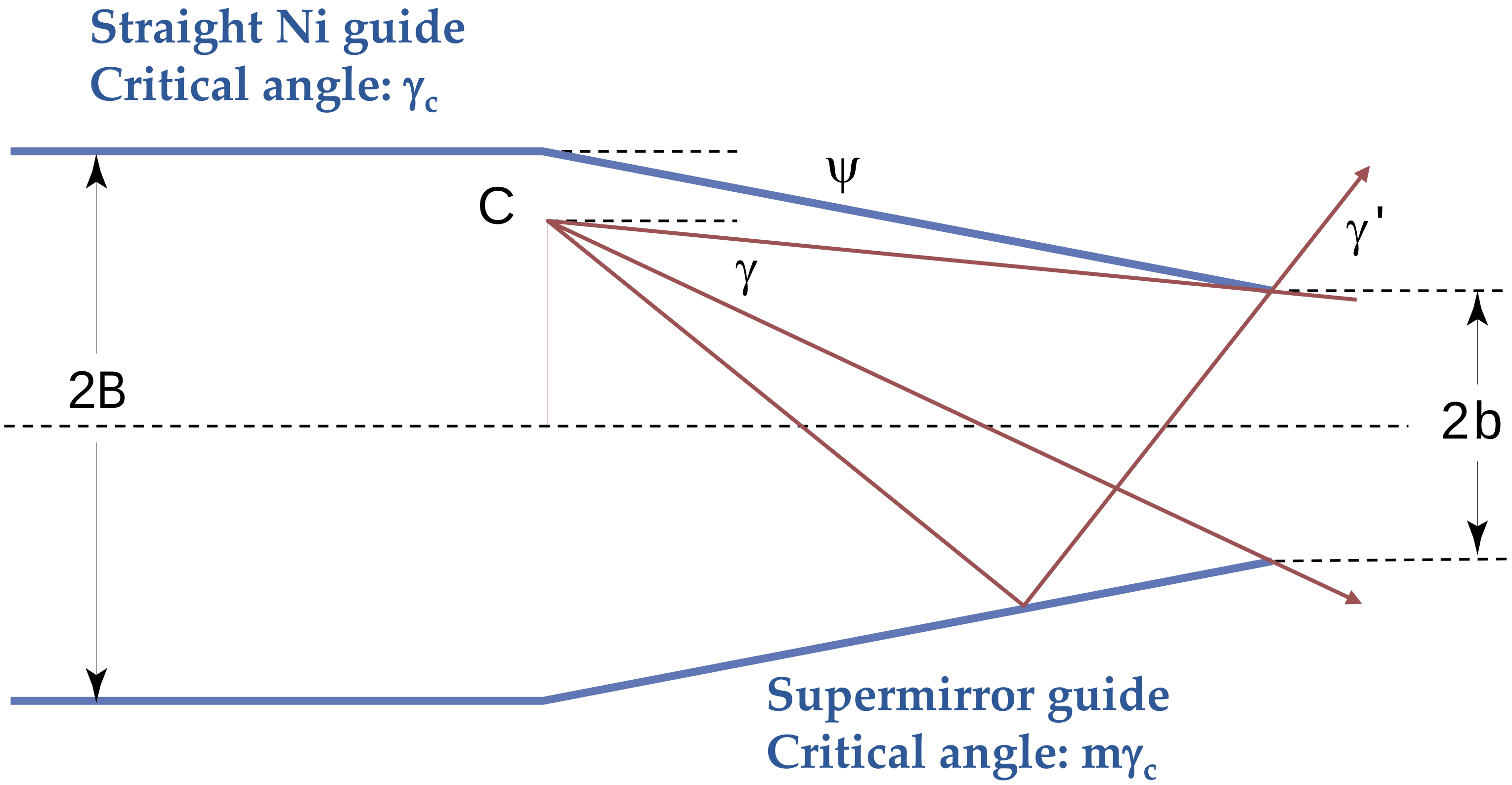
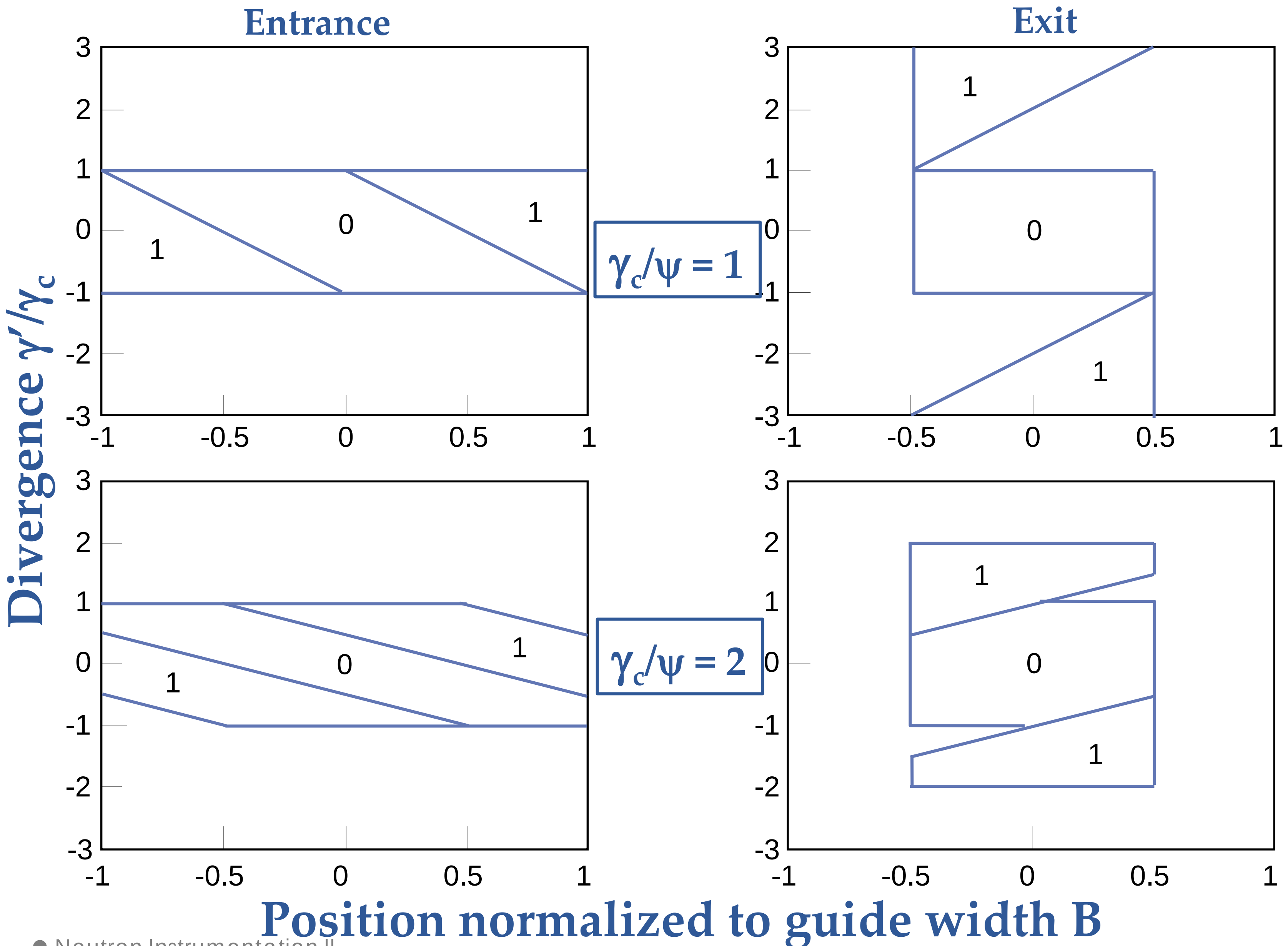
Converging Neutron Guides

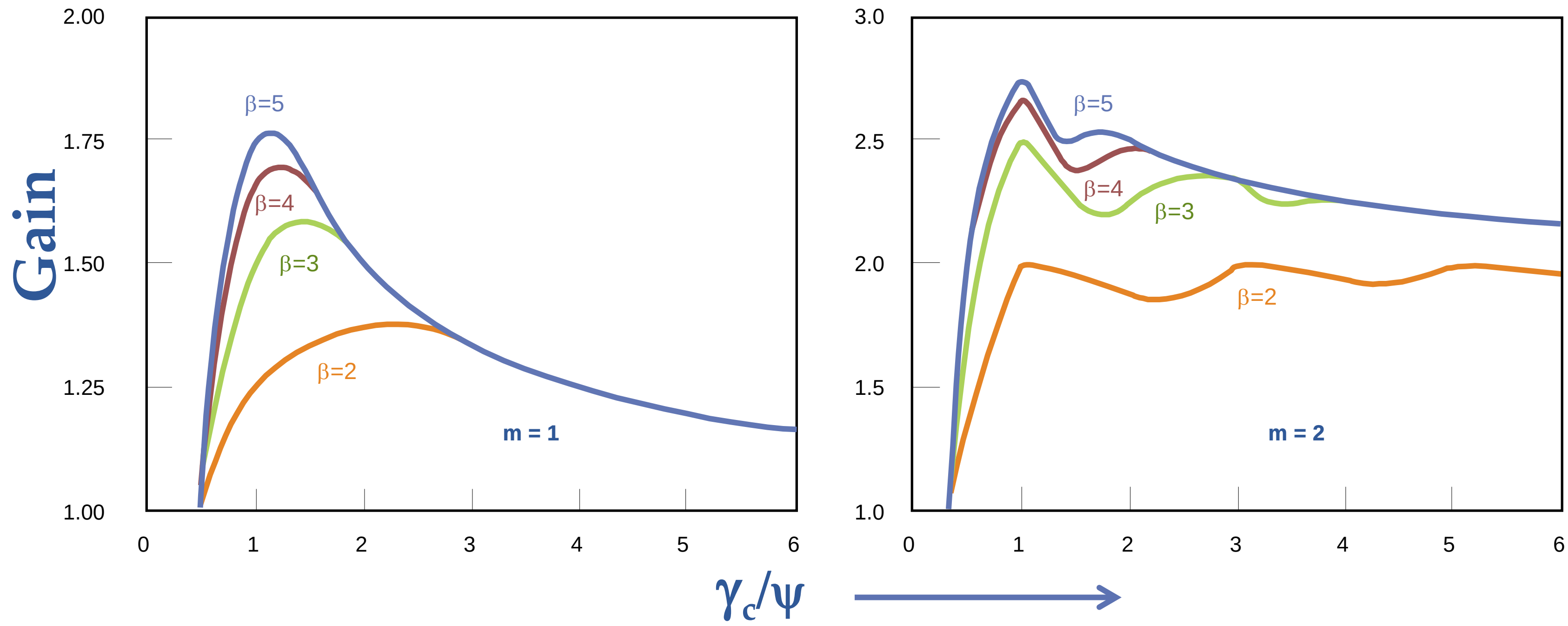


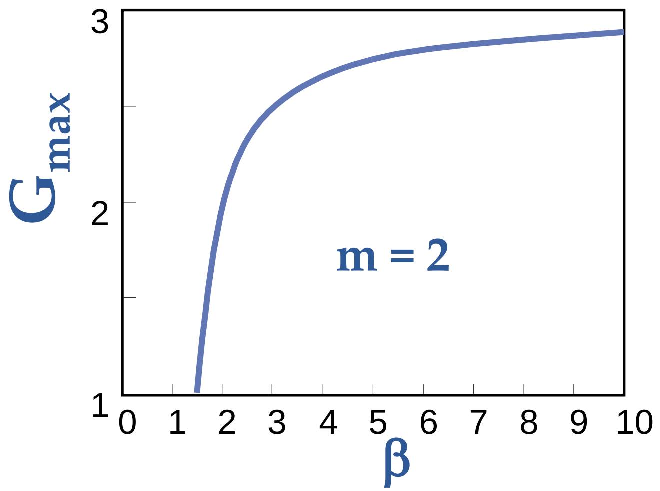
Liouville: Focusing in real space ($\beta = B/b$) must be associated with increase in divergence

Phase space picture (m=2, β=2)



Effective gain in flux

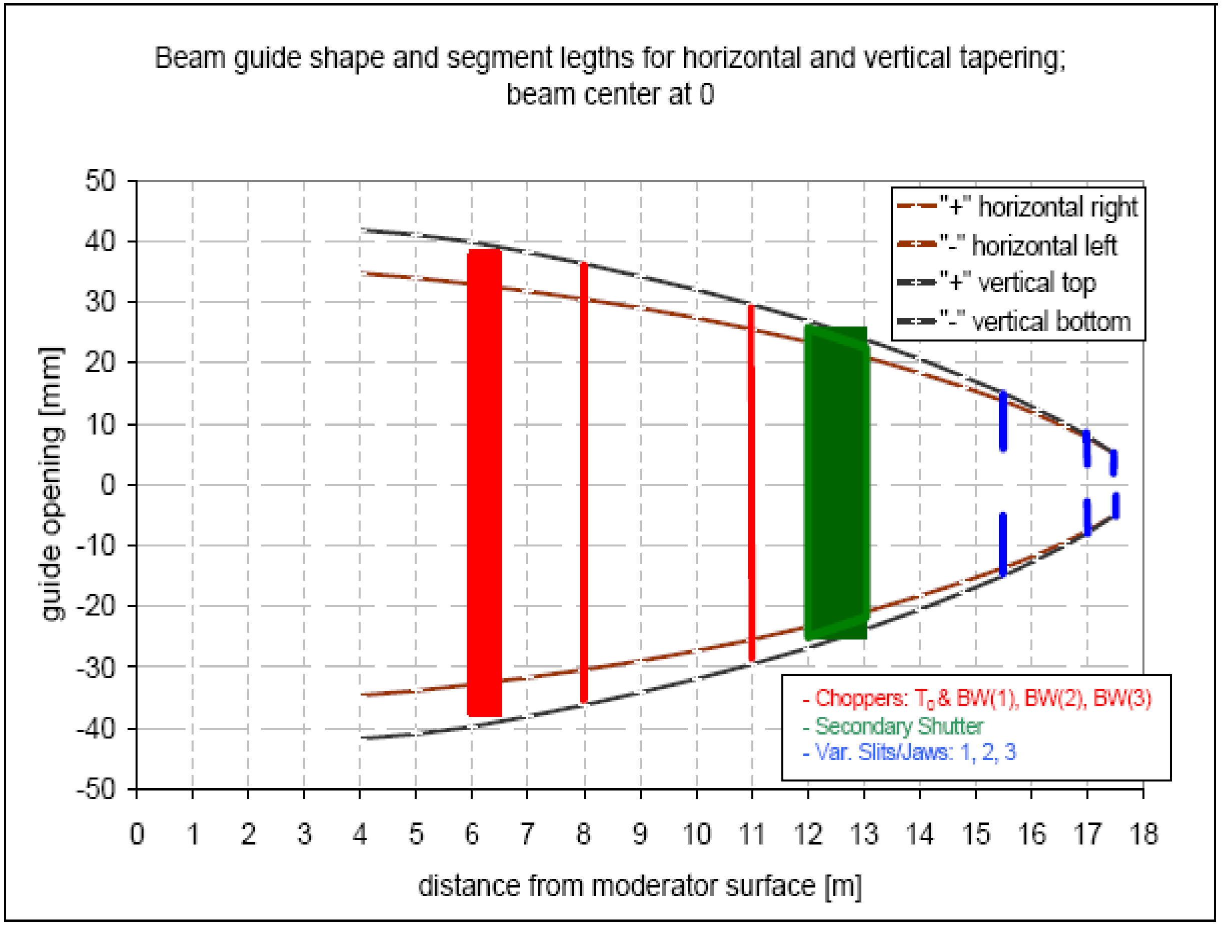




Some interesting facts:

- For $\beta \leq m$, Gain = m
- Maximum gain $G_{max} = 1 + m$
  - only reached at infinite β

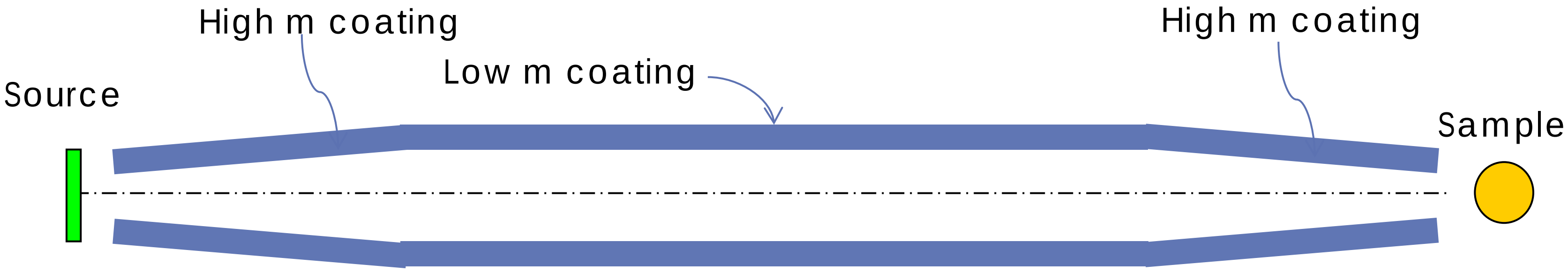
It can be more complicated!



Guide design for the TOPAZ instrument at SNS

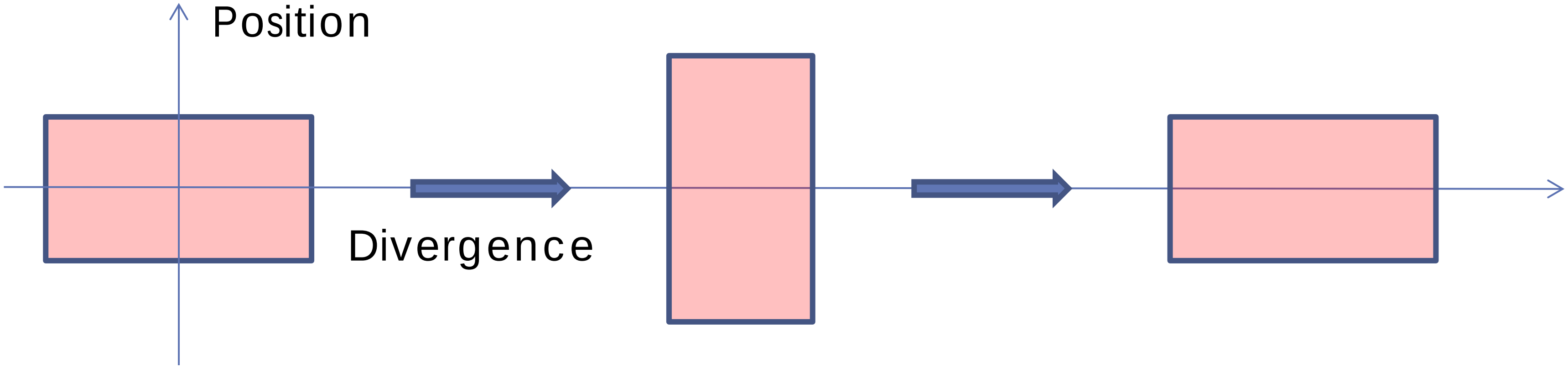
Ballistic guides

An efficient way of transporting neutrons with low losses



A simple ballistic guide

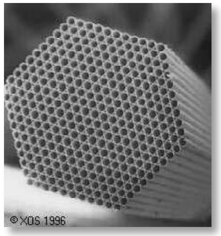
In phase space

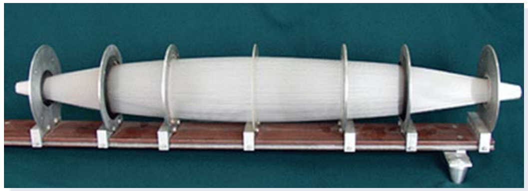


Fewer reflections at lower angle -> higher transmission

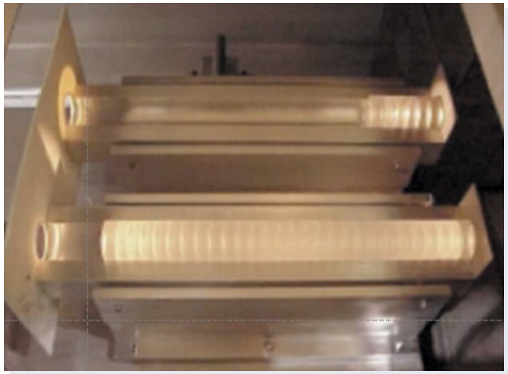
Some things we didn't talk about:

- Capillary Optics

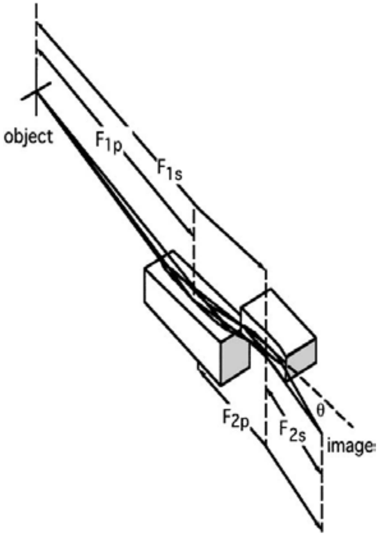




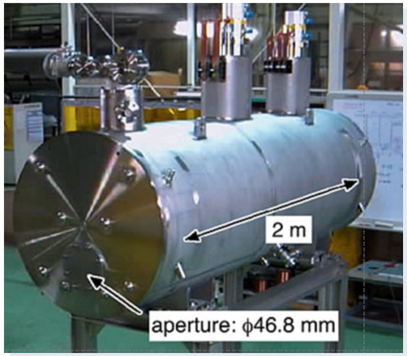
- Compound Refractive Lens



- Elliptical mirrors



- Polarized Neutrons (next installment)
- Magnetic Lens



Summary

- For many instruments natural collimation does not accept all the angular divergence that could be used in the experiment – angular resolution is too good
- Neutron Guides can be used to transport neutrons over quite long distances
- Supermirrors are commonly used to increase the transmitted divergence
- Focusing obeys Liouville!

Thank you!