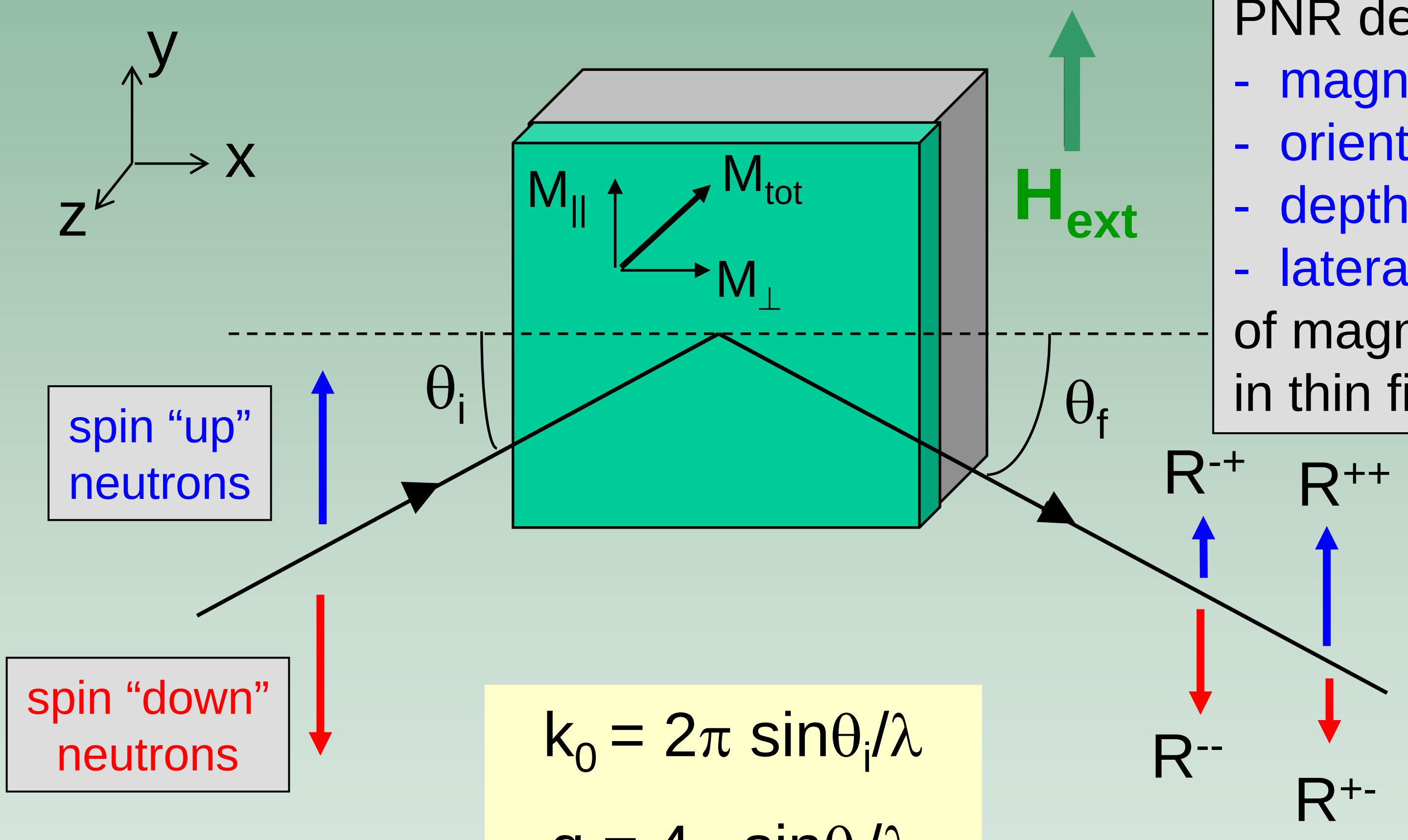
Introduction to Polarized Neutron Reflectometry

Frank Klose
Instrument Scientist
Oak Ridge National Laboratory

SNS/HFIR User Meeting

October 13, 2005

Polarized Neutron Reflectometry



PNR determines:
- magnitude
- orientation
- depth distribution
- lateral arrangements

of magnetization vectors in thin film structures

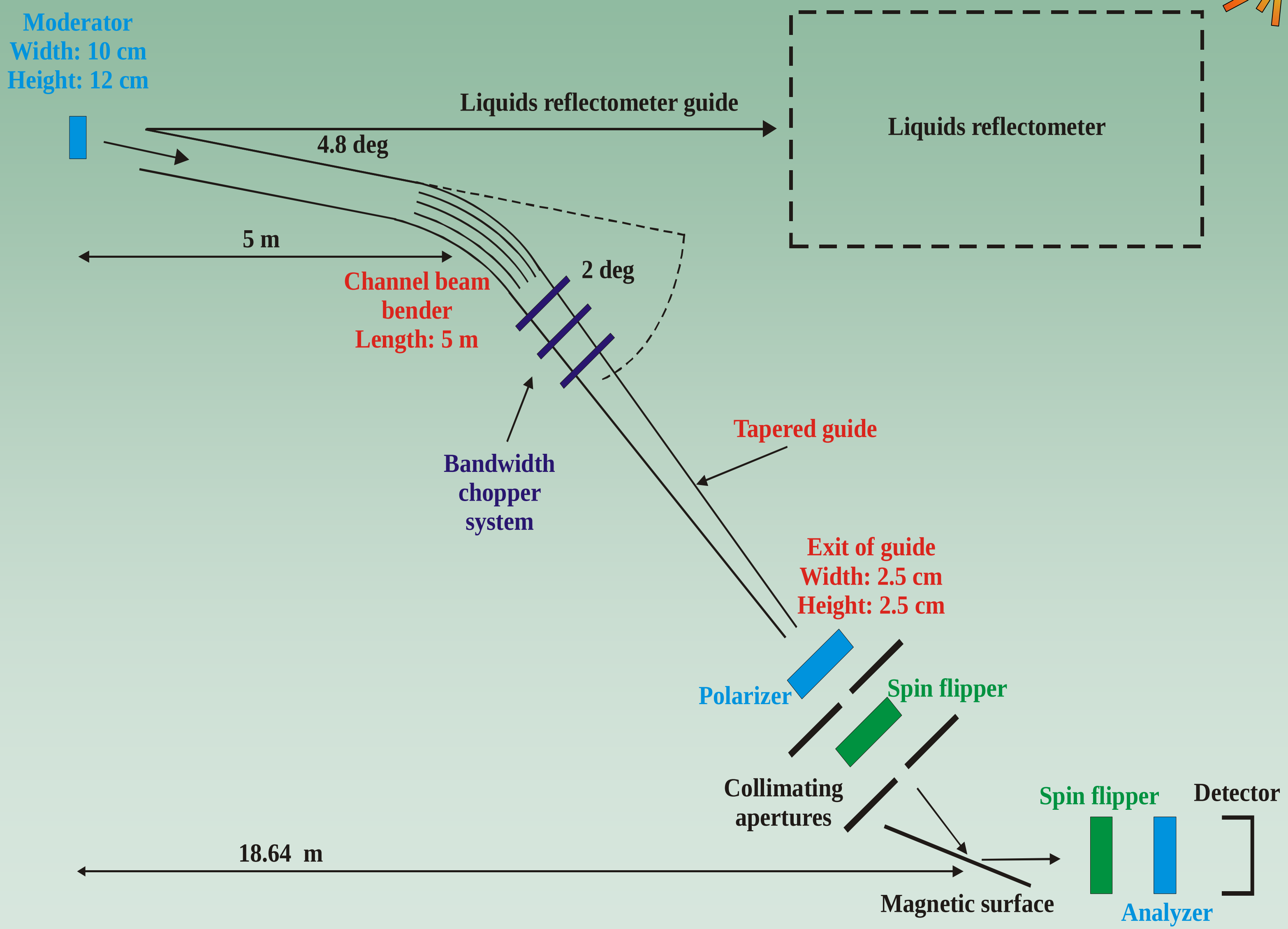
$$k_0 = 2\pi \sin\theta_i/\lambda$$

$$q = 4\pi \sin\theta_i/\lambda$$

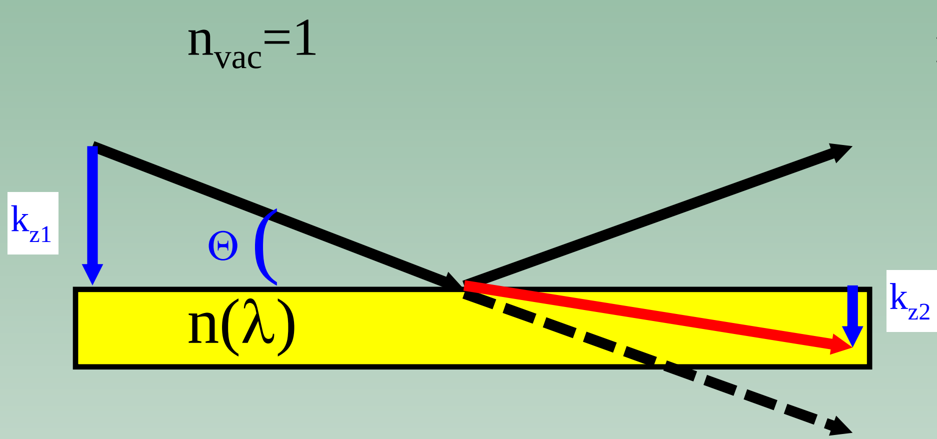
measurement of **four** cross-sections

Frank Klose *Email: KloseFR@ornl.gov*

The SNS Magnetism Reflectometer - Schematic



Total Reflection at Surfaces



For neutrons (and X-rays) with wavelengths of a few Å, almost all materials have an optical index slightly smaller than 1.

=> Total reflection up to a critical angle $\Theta_{crit}(\lambda)$

Refraction index:

$n(\lambda) = k_{z2}$ (inside the media) / k_{z1} (outside)

Kinetic energy of a free particle:

$E_1 = \hbar^2 k_{z1}^2/2m_N$

Inside the media with potential V, k_{z2} is (in most cases) smaller (conservation of energy):

$\hbar^2 k_{z2}^2/2m_N + V = E_1$

$\Rightarrow \quad k_{z2} = (k_{z1}^2 - 2m_N V/\hbar^2)^{1/2}$

Connection to microscopic properties:

Fermi pseudo potential: $V = 2\pi \hbar^2 N b/m_N$

with N: number density [at/cm^3]
b: coherent scattering length of the nuclei in the material [fm]

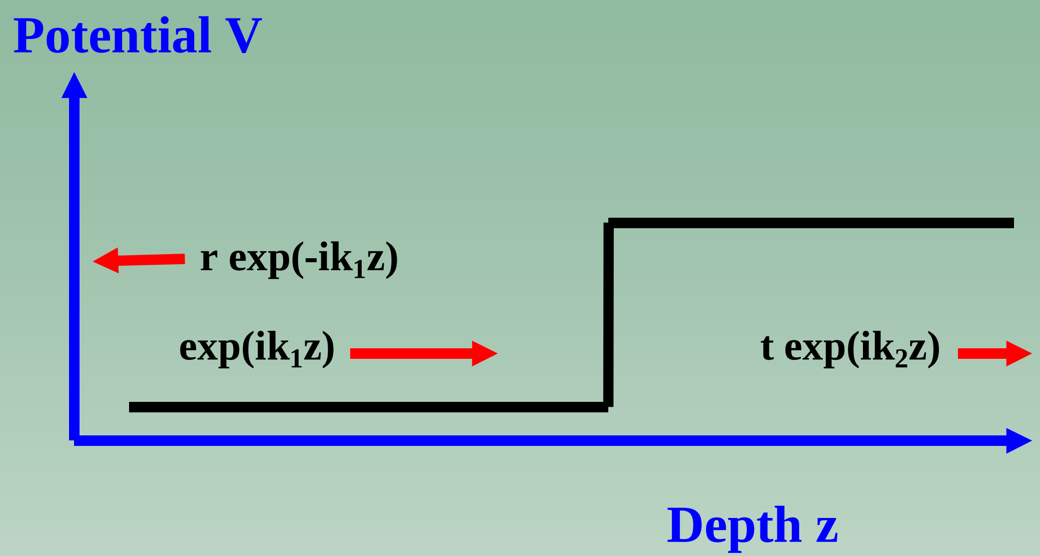
Critical angle for total reflection is reached, if E_z=V !

$\Theta_{crit} = \sin^{-1}\lambda(N\cdot b/\pi)^{1/2} = \cos^{-1} n$

or

$Q_{crit} = 4\pi \sin\Theta/\lambda = 4(\pi N\cdot b)^{1/2}$

Calculation of the Reflectivity at a Potential Step



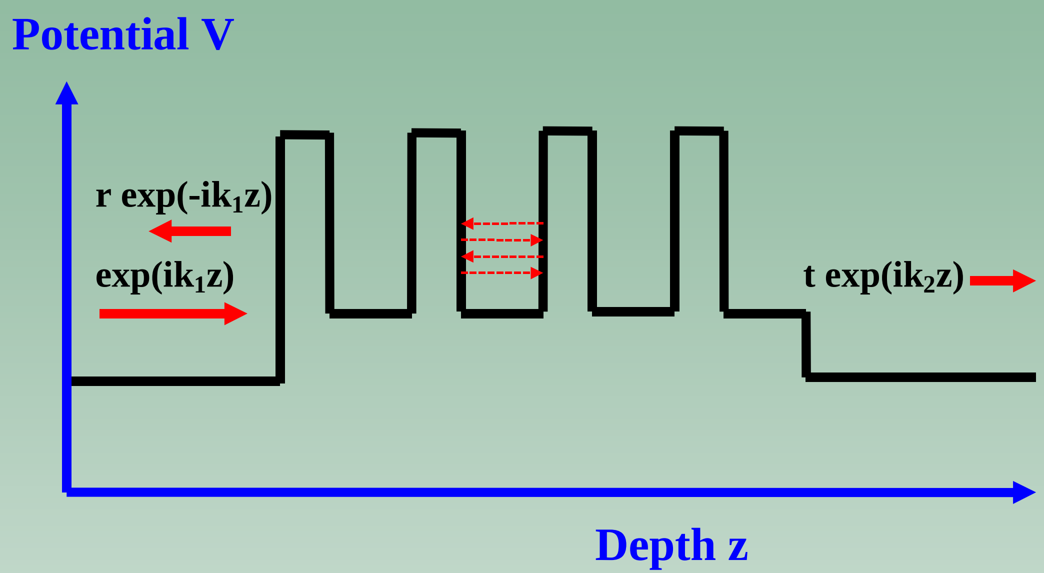
Solution of the quantum mechanic problem:

Fresnel equations

Reflectivity $R = |r|^2 = |(k_1 - k_2) / (k_1+k_2) \exp(i2k_1z)|^2$

Transmission $T = |t|^2 = |2k_1 / (k_1+k_2) \exp(i2(k_1 - k_2)z)|^2$

Example: Potential of a Multilayer



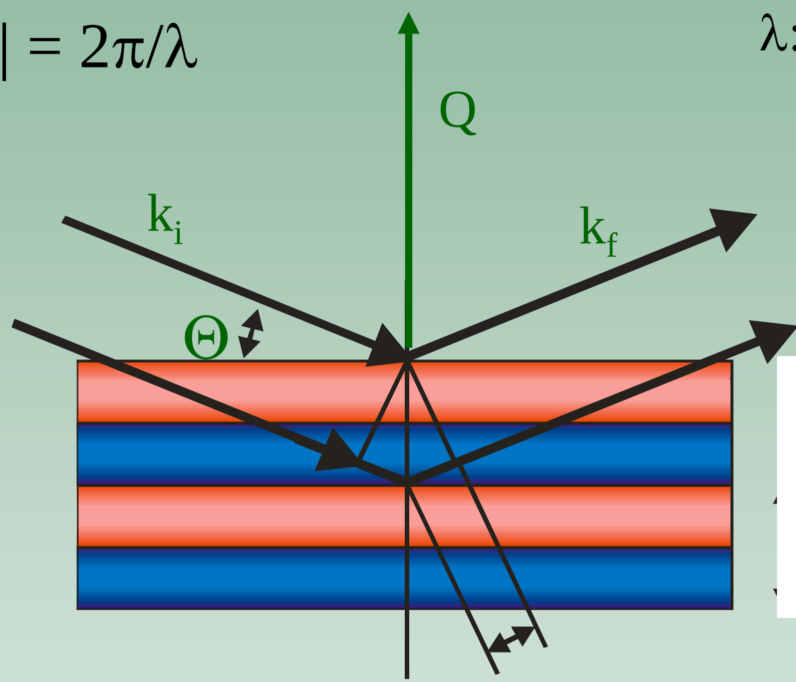
At each interface one has to take into account:

- Refraction effects
- Multiple-scattering effects

Neutron Reflectivity

$|\mathbf{k}| = 2\pi/\lambda$

Θ: angle of incidence
λ: wavelength



The reflectivity of the sample is measured as a function of the scattering vector Q

$\mathbf{Q} = -\mathbf{k}_i + \mathbf{k}_f$
$|\mathbf{Q}| = 4\,\pi \sin\Theta / \lambda$

=> two concepts for neutron reflectivity measurements:

a) fixed wavelength + variable angle
b) variable wavelength + fixed angle

Bragg's Law for Periodic Layered Structures

constructive interference if: $2d \sin\Theta = n\,\lambda$

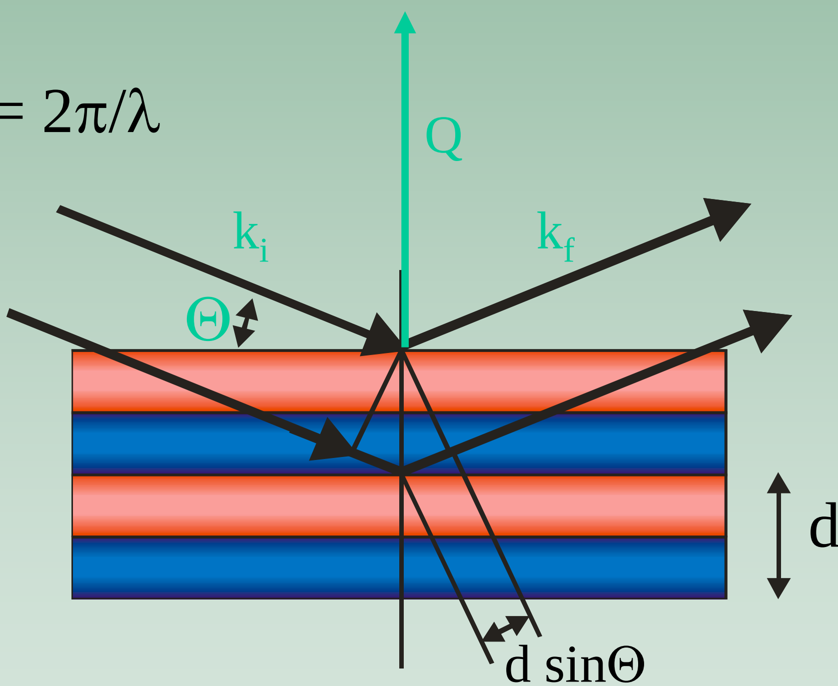
d: double layer thickness

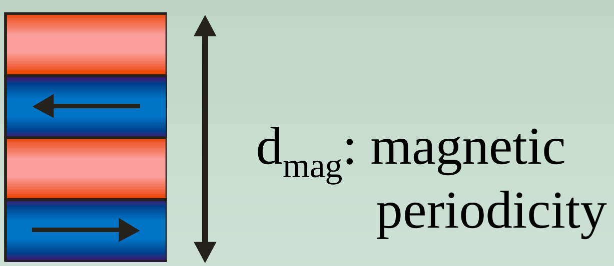
Θ: angle of incidence

n: order number (0,1,2,...)

λ: wavelength

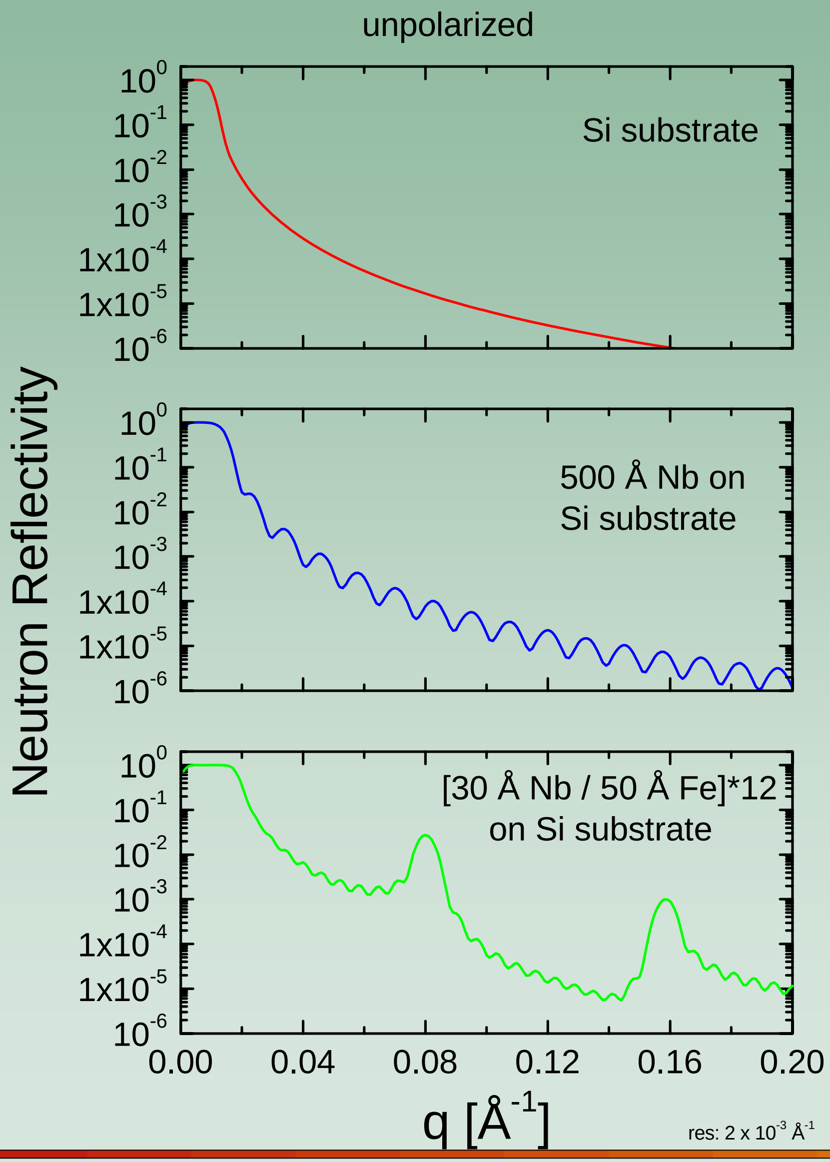
$|\mathbf{k}| = 2\pi/\lambda$

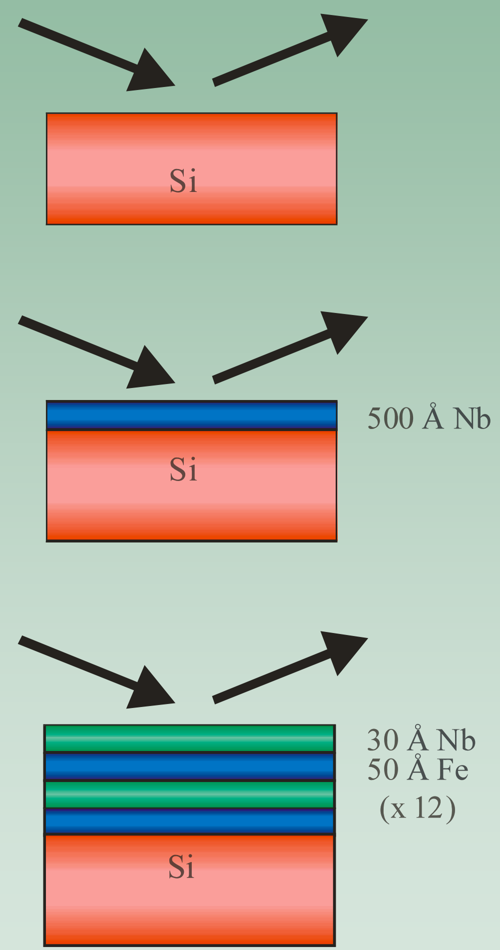




example:
antiferromagnetic coupling
of magnetic layers

Reflectivity of Layered Structures





What are Polarized Neutron Beams ?

The neutron:

spin 1/2 particle (Fermion)

=> its component along a given direction z can only be "up" (+) or "down" (-)

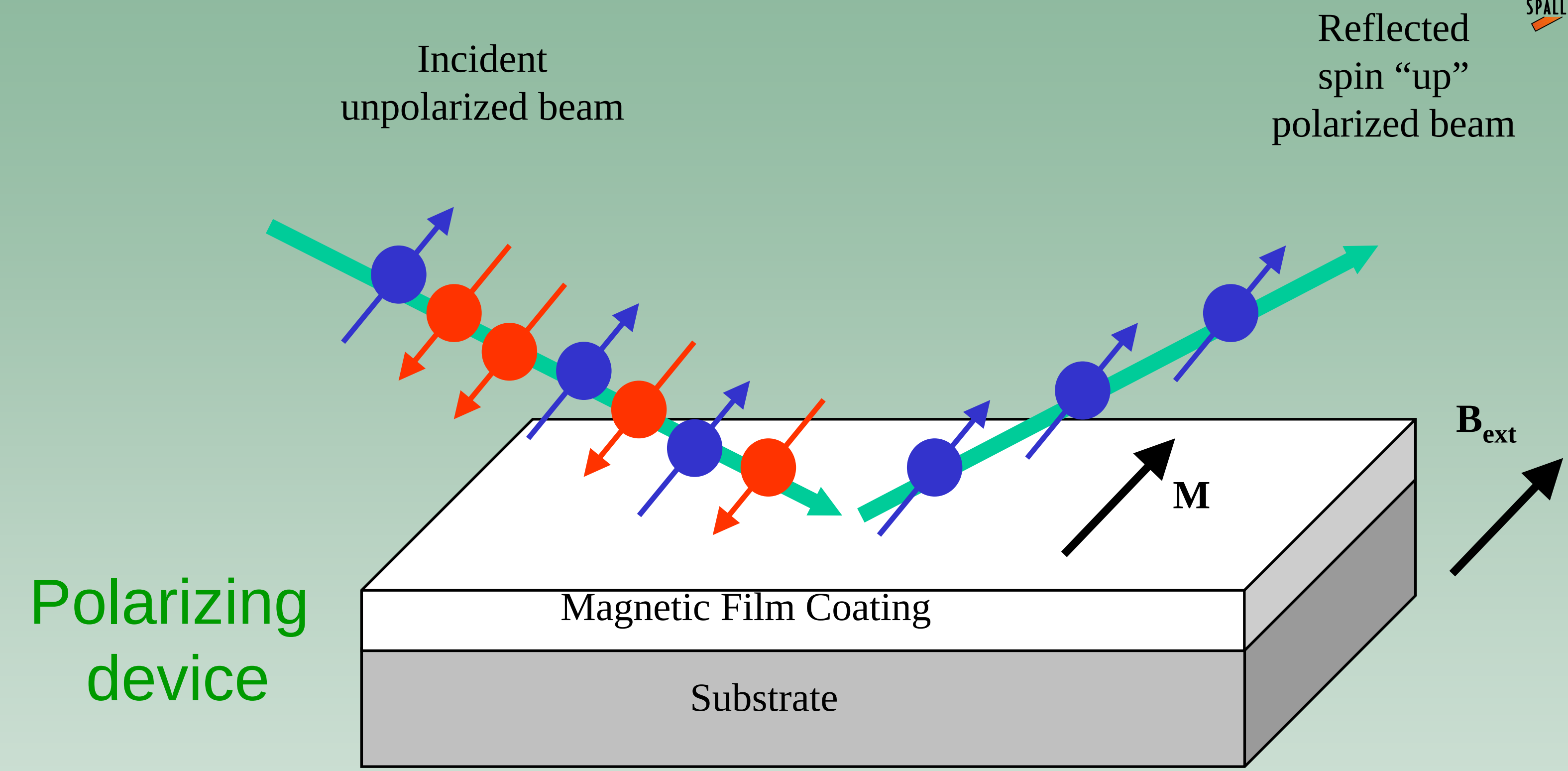
Nuclear magnetic dipole moment:

μ_N = -1.913 nuclear magnetons = 5.4 x 10^{-4} μ_B

(comparison: Fe atom = 2.2 μ_B)

=> neutrons have strong direct interaction with atomic and nuclear spins

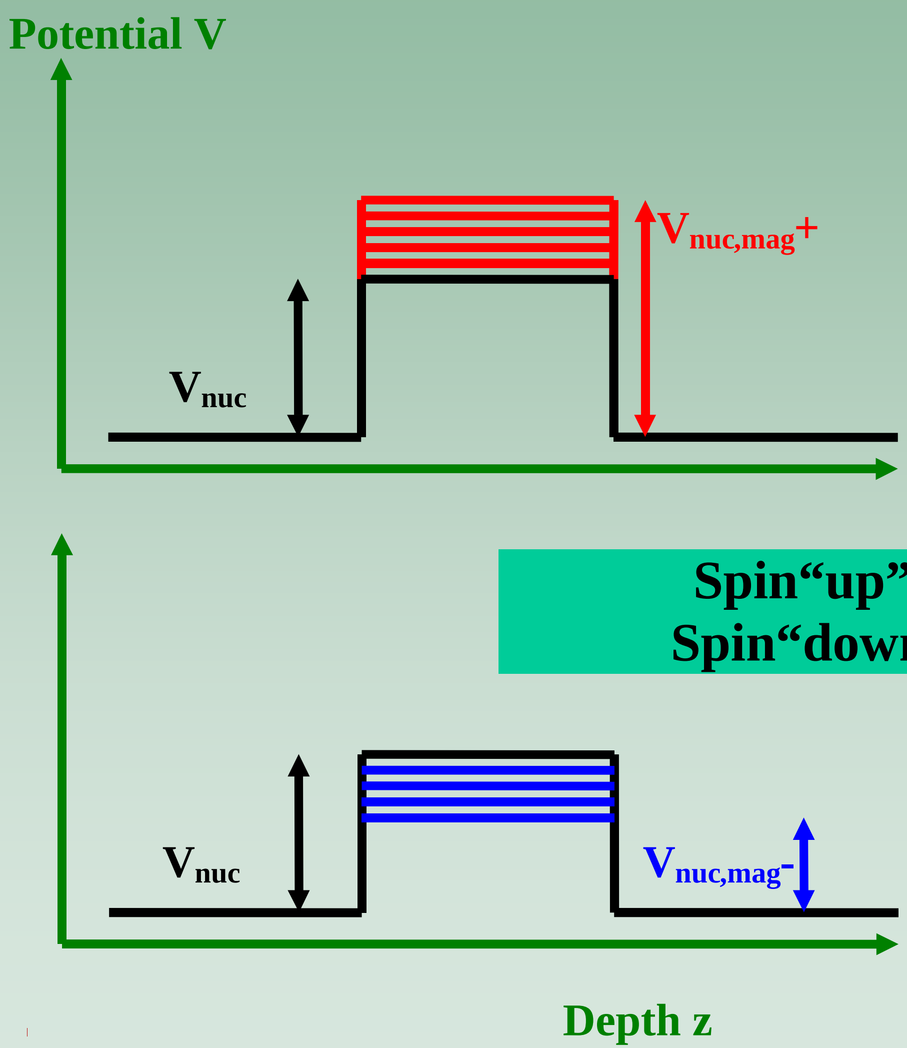
What are Polarized Neutron Beams ? - Cont'd



Beam Polarization *P*: $$P = \frac{N_{up} - N_{down}}{N_{up} + N_{down}}$$ => **0 < |*P*| < 1**

N_{up} (N_{down}): number of "up" ("down") neutrons in the beam

Neutron Reflectivity on a Single Magnetic Layer

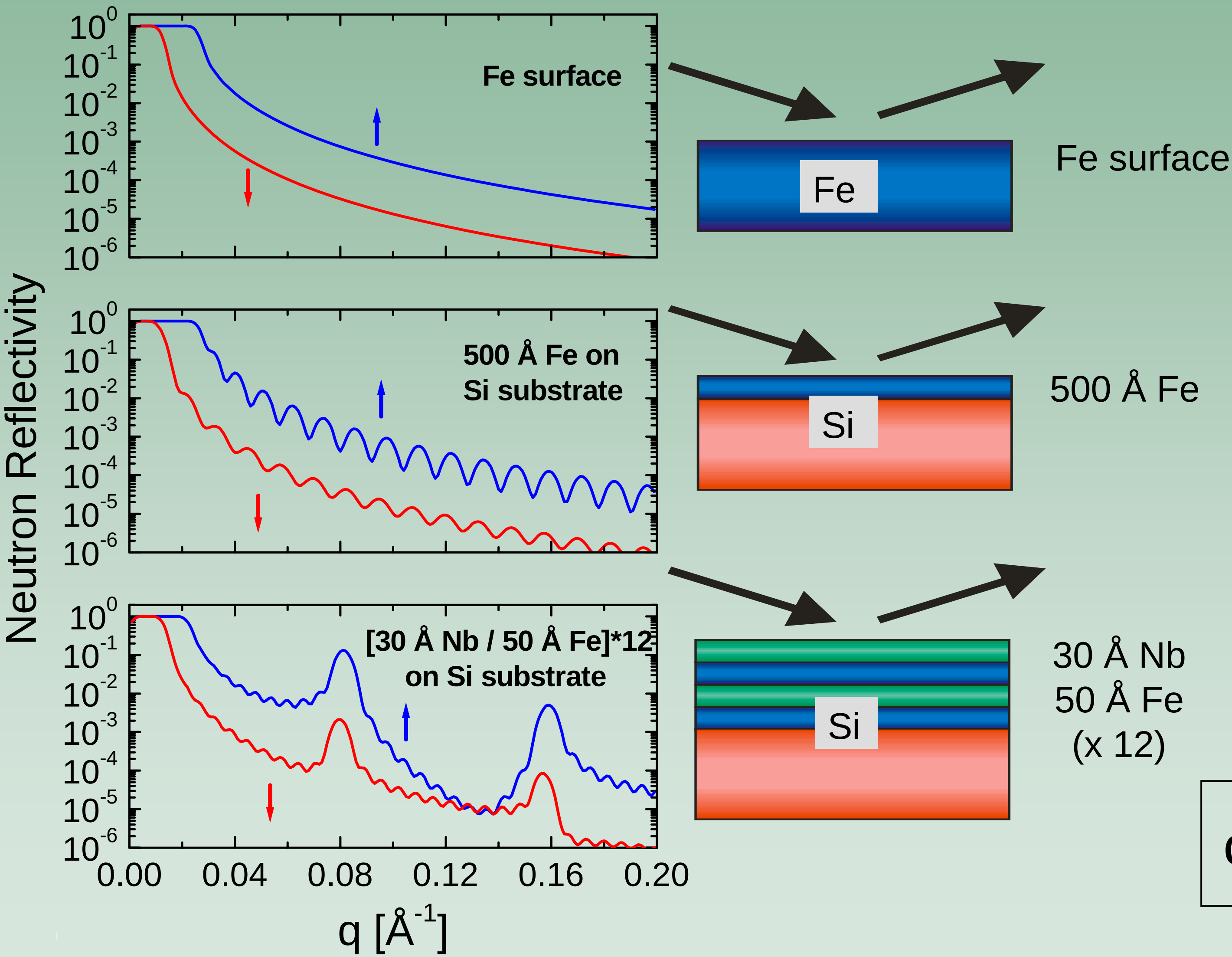


Fermi pseudo potential:
$V = 2\pi \hbar N (b_{nuc} +/- b_{mag})/m_N$

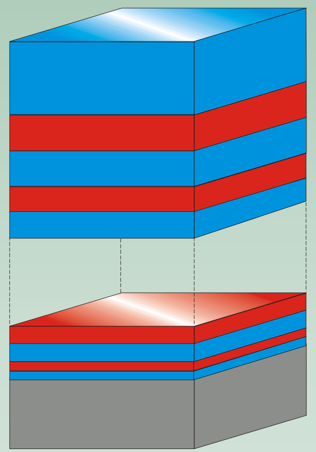
b_{nuc}:	nuclear scattering length [fm]
b_{mag}:	magnetic scattering length [fm] (1 μ_B/Atom => 2.695 fm)
N:	number density [atoms/cm^3]
m_N:	neutron mass

Spin "up" neutrons see a high potential.
Spin "down" neutrons see a low potential.

Polarized Neutron Reflectivity of Layered Magnetic Structures



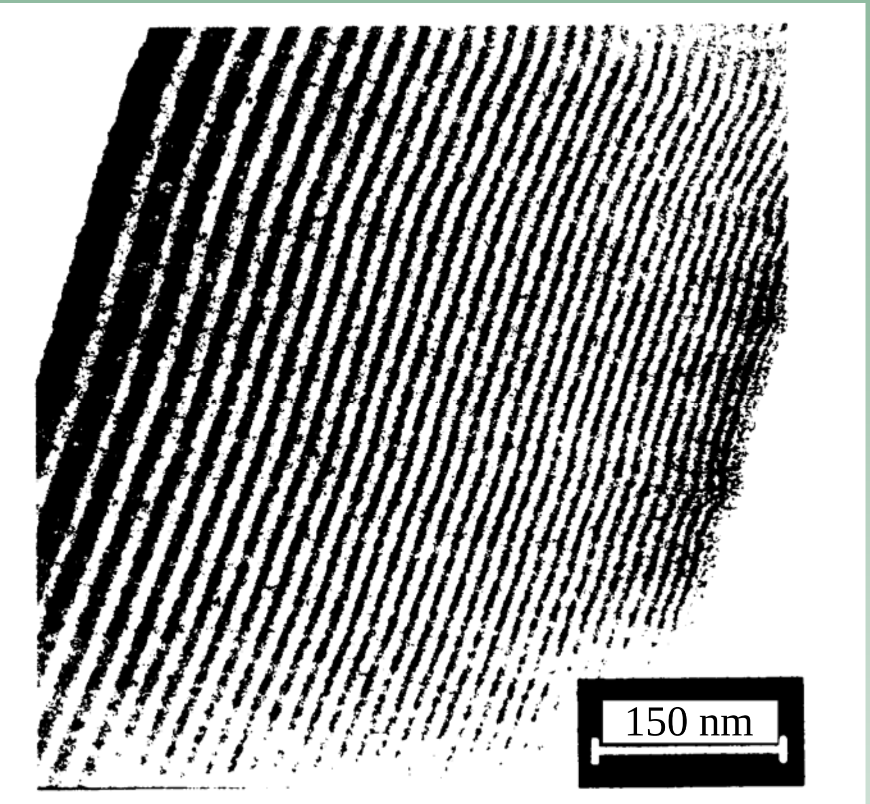
Supermirror (Mezei)

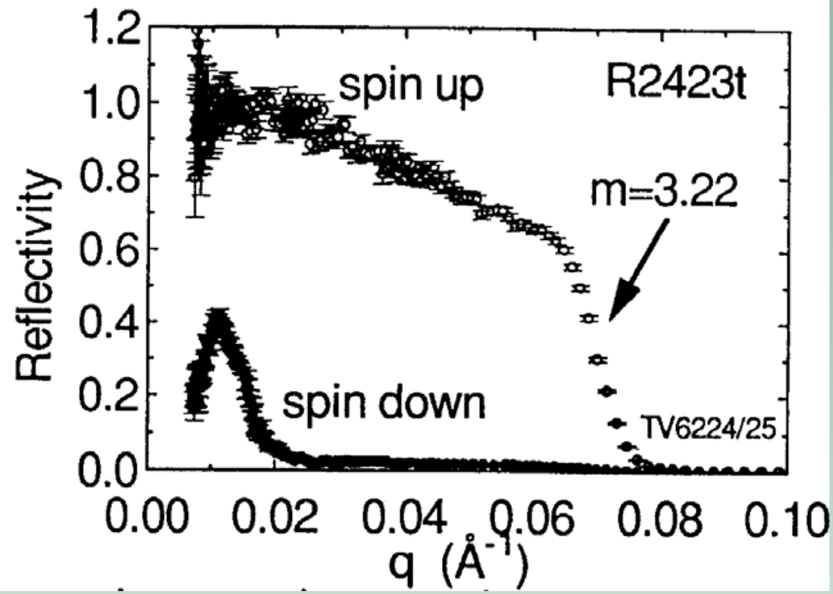


$$q_c^{SM} = m \times q_c^{Ni}$$

SNS Instrument Systems *Frank Klose* *Email: KloseFR@ornl.gov*

Polarizing Supermirrors



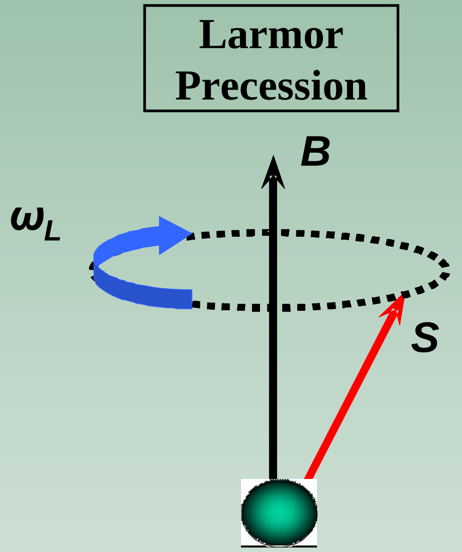


Scattering length densities of non-magnetic layer and magnetic layer (spin-down) must match
=> no reflection of spin-down neutrons

State-of-the-art polarizing supermirror:
$Fe_{50}Co_{48}V_2/TiN_x$
Reflectivity = 80% for spin "up" neutrons at 3 times critical q of natural Ni
P. Boeni, Physica B 234-236 (1997) 1038

Spin Flippers – Larmor Precession

The time evolution of the expectation value of the spin of a spin-1/2 particle in a magnetic field can be determined classically as:



Courtesy:
R. Pynn

$$\frac{d}{dt}\mathbf{s}(t) = \gamma[\mathbf{s}(t) \times \mathbf{B}(t)]$$

$$\Rightarrow \quad \omega_L = \gamma B$$

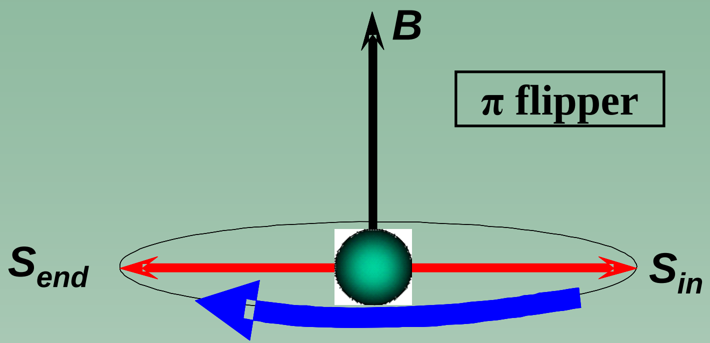
$$\gamma/2\pi = -2916.4\ \text{Hz/G}$$

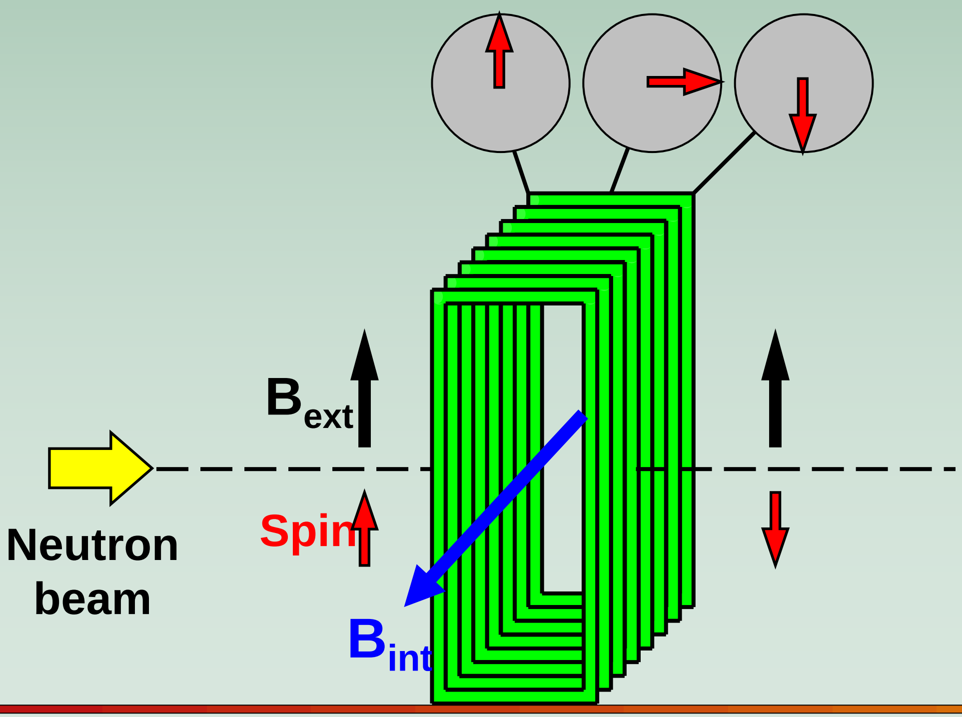
$\gamma/2\pi$: gyromagnetic ratio of the neutron,
B: magnetic field vector
S: spin vector of the neutron
ω_L: Larmor frequency

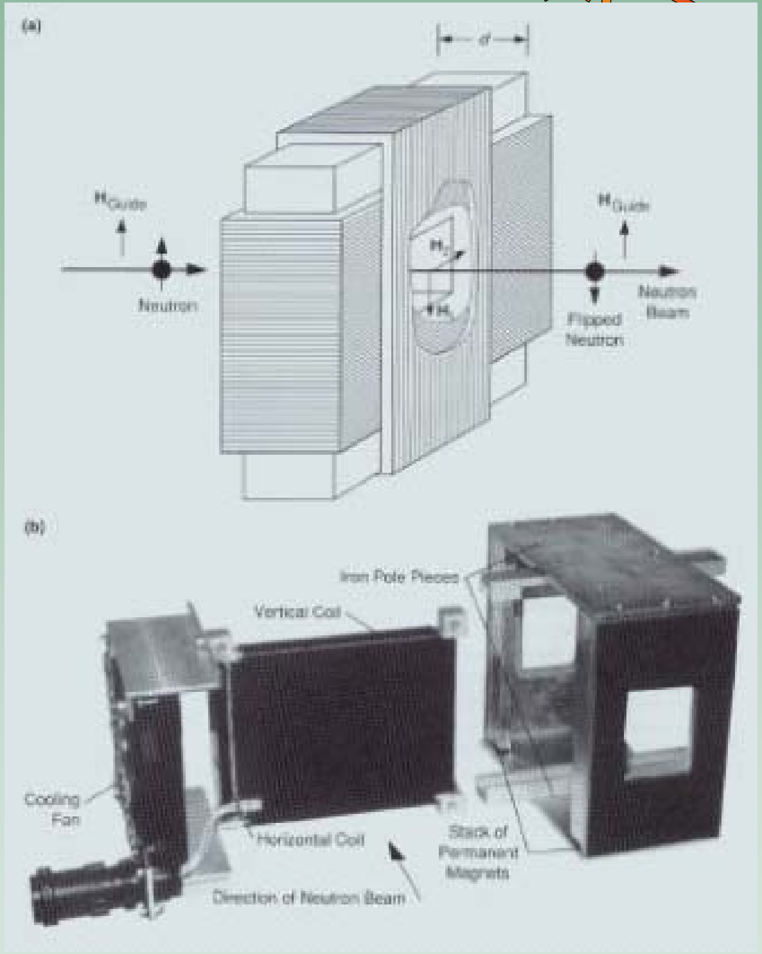
The total precession angle of the spin, Φ, depends on the time the neutron spends in the field: $\Phi = \omega_L * t$ Example:

B (Gauss)	ω_L(rad/sec)	$v_{Neutron}$ (m/sec) for 4 Å neutrons	Turns (per 1 m) for 4 Å neutrons
10	183000	989	29

π Spin Flipper: *Mezei* Spin Flipper

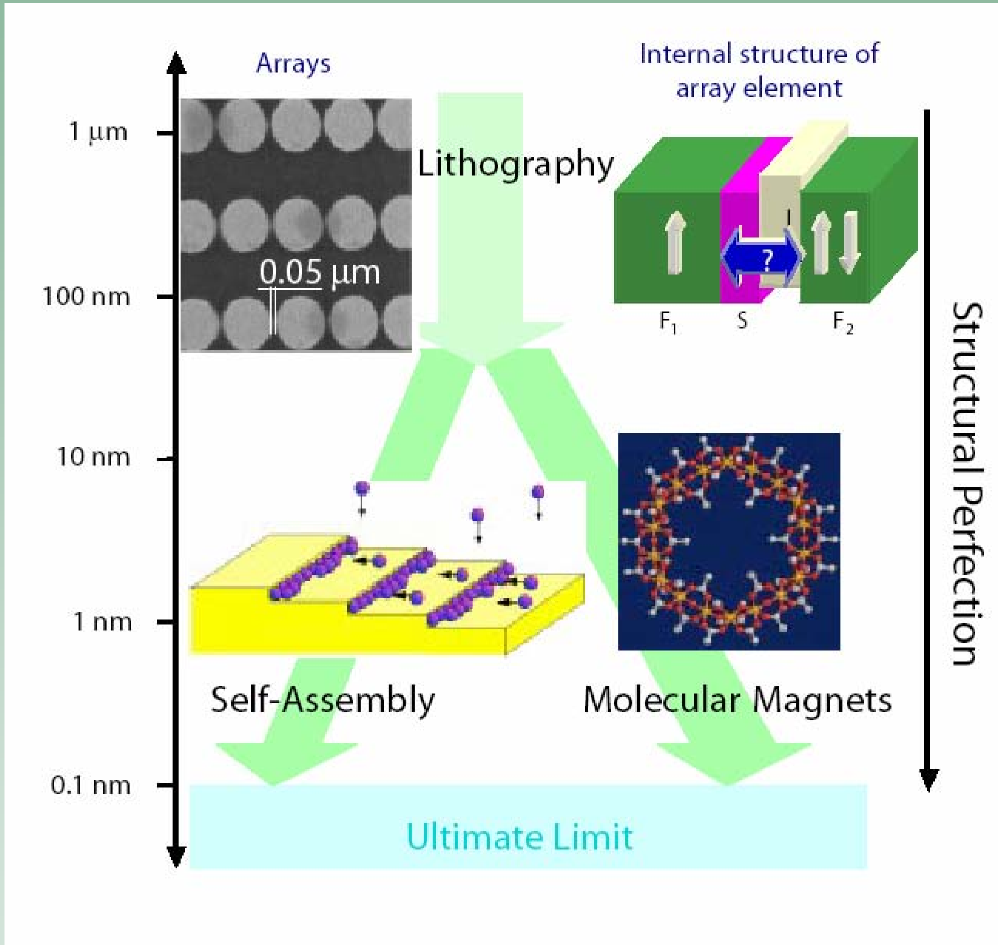






Number of spin turns N:
N = 1/135.65 * B (Gauss) * d (cm) * λ (Å)

Polarized Reflectometry:
- Science Examples



From:
Complex Systems: Science for the 21st Century
Laterally Confined Nanomagnets
D. Argyriou, S.D. Bader, D. Li, H.H. Wang, and U. Welp

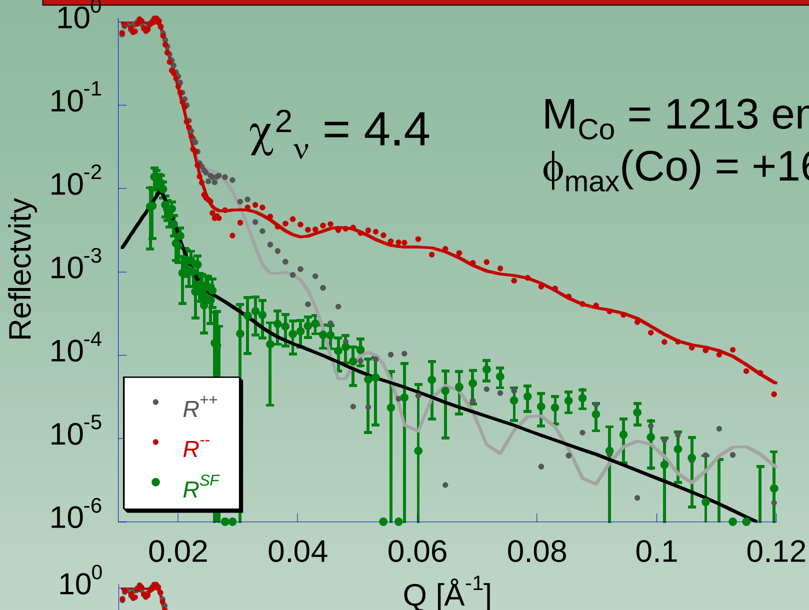
>10's of micron to micron (10^{-4} – 10^{-6} m):
– Magnetic domains

Micron to Submicron (10^{-6} – 10^{-8} m):
– Magnetic interactions in lithography samples (magnetic storage)

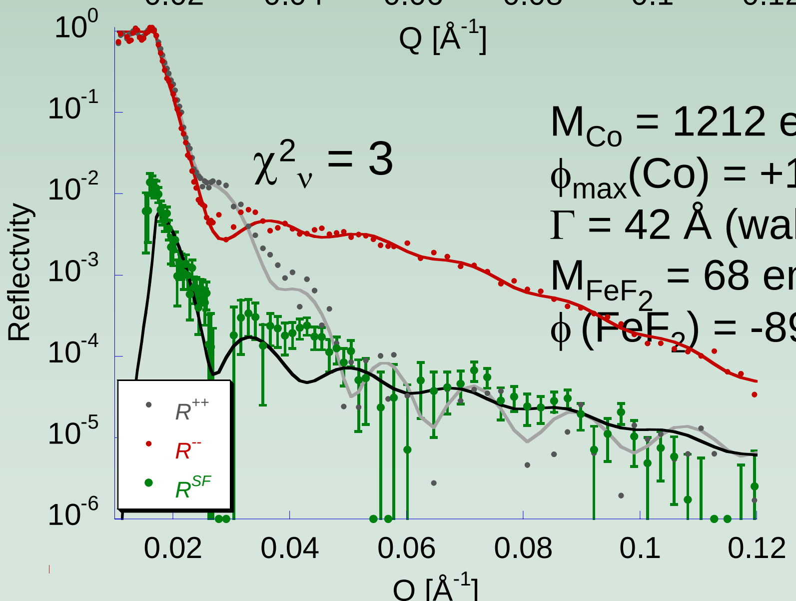
Submicron to Nano (10^{-7} – 10^{-9} m):
– RKKY coupling in magnetic multilayers (giant magnetoresistive films)

Nano to Angstrom (10^{-9} – 10^{-10} m):
– Ultrathin magnetic films

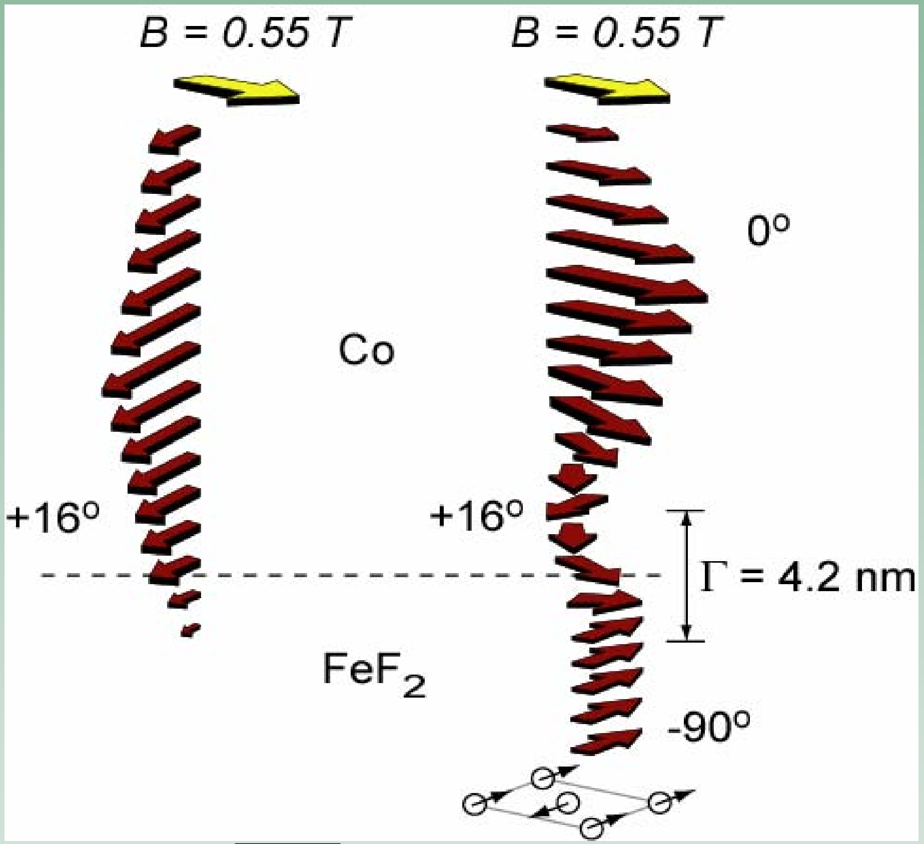
Magnetic Coupling at Exchange Bias Interfaces: Twisted or Fan Magnetic Structures



M_{Co} = 1213 emu/cm^3
ϕ_{max}(Co) = +16^o



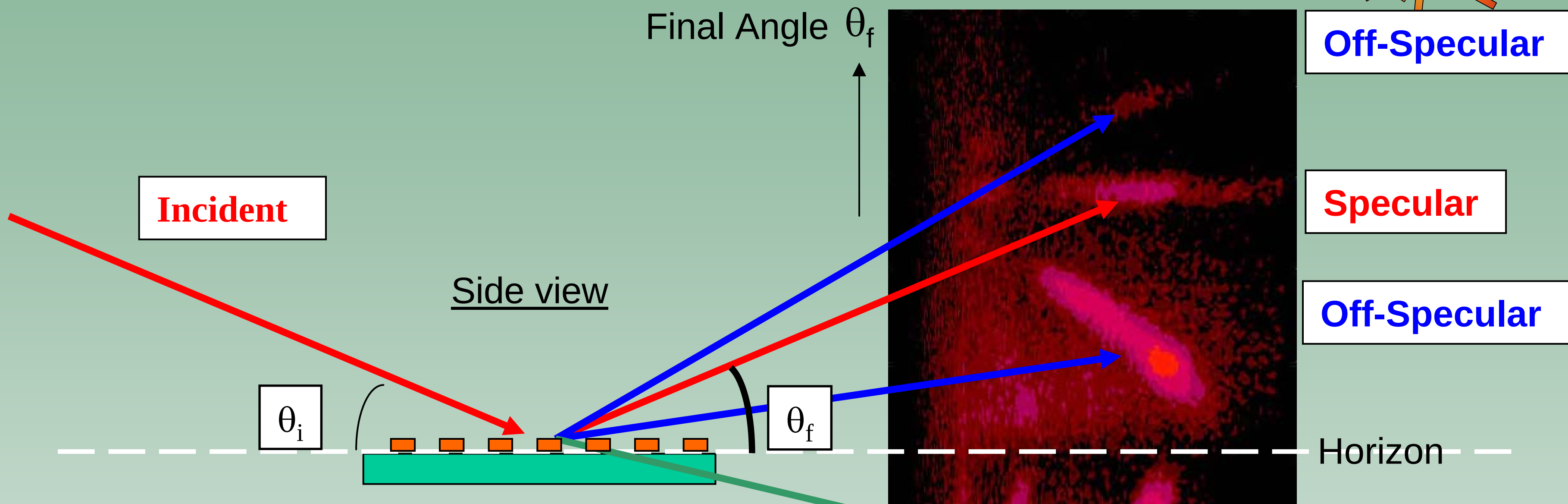
M_{Co} = 1212 emu/cm^3
ϕ_{max}(Co) = +16^o
Γ = 42 Å (wall width)
M_{FeF_2} = 68 emu/cm^3
ϕ (FeF_2) = -89^o

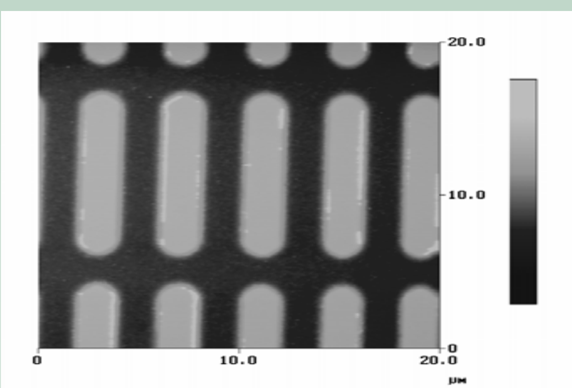


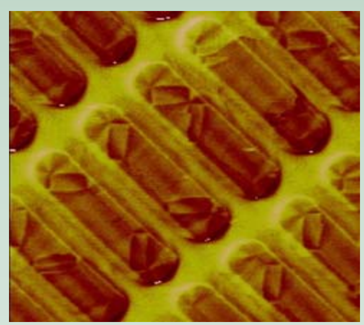
$$\Gamma = \frac{\pi}{2}\sqrt{\frac{J}{Ka_0}} \Rightarrow K_{\text{int}} \approx 10^6 erg/cm^3$$

Courtesy: M. Fitzsimmons

Example: Off-Specular Scattering From Lateral Structures



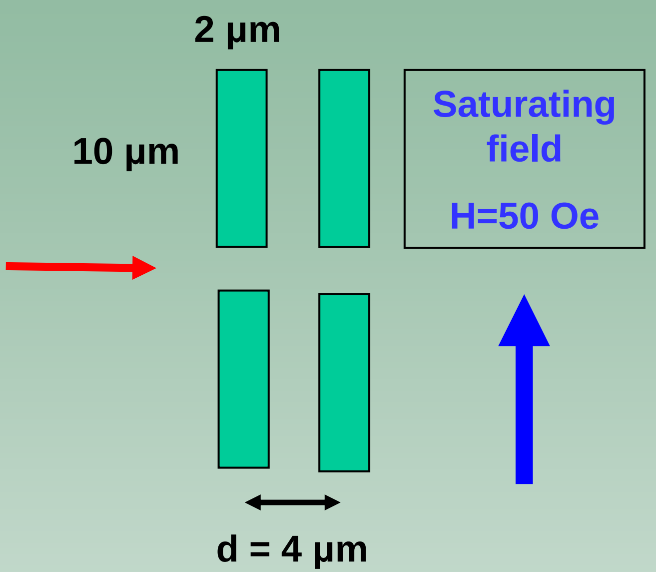


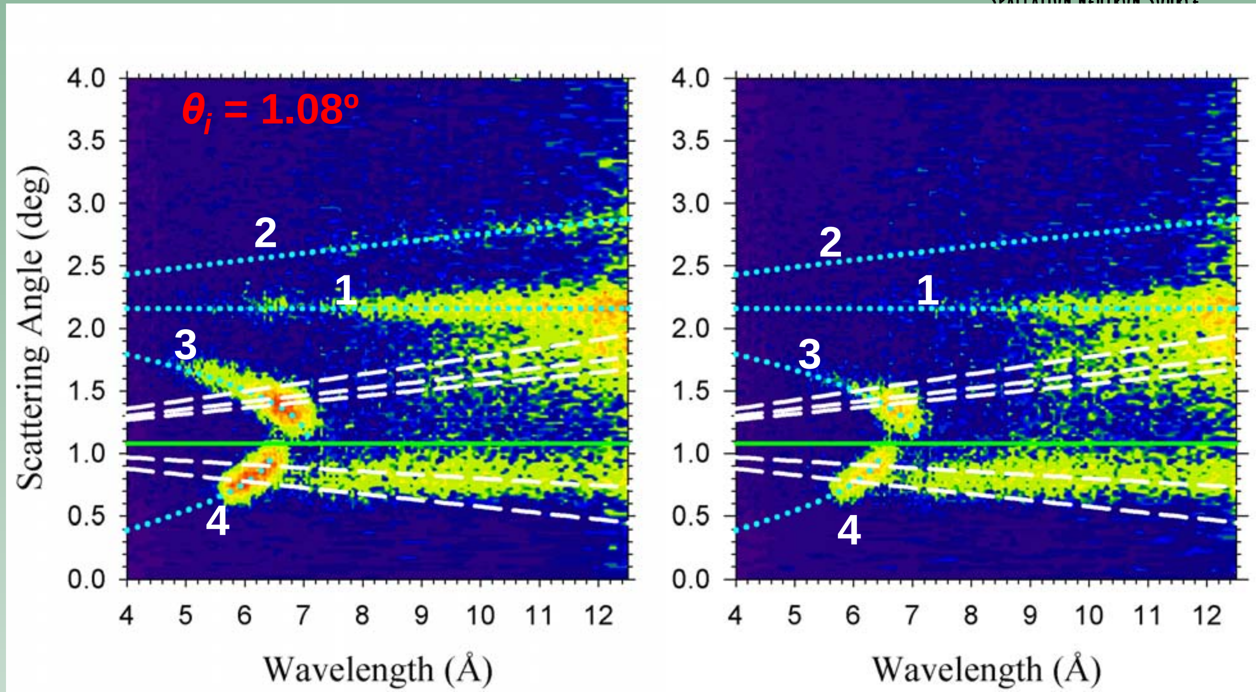


Sample: 10µm x 2µm Ni stripes (100 Å film thickness)

W.T. Lee & F. Klose, 2002

Polarized Neutron Time-Of-Flight Off-Specular Scattering





(Intensities are normalized to the incident spectrum)

1: specular reflection

2,3: off-specular reflections (above horizon)

$$\theta = \theta_i + \sqrt{\theta_i^2 + 2n\lambda / d} \quad \text{with } n = +/- 1$$

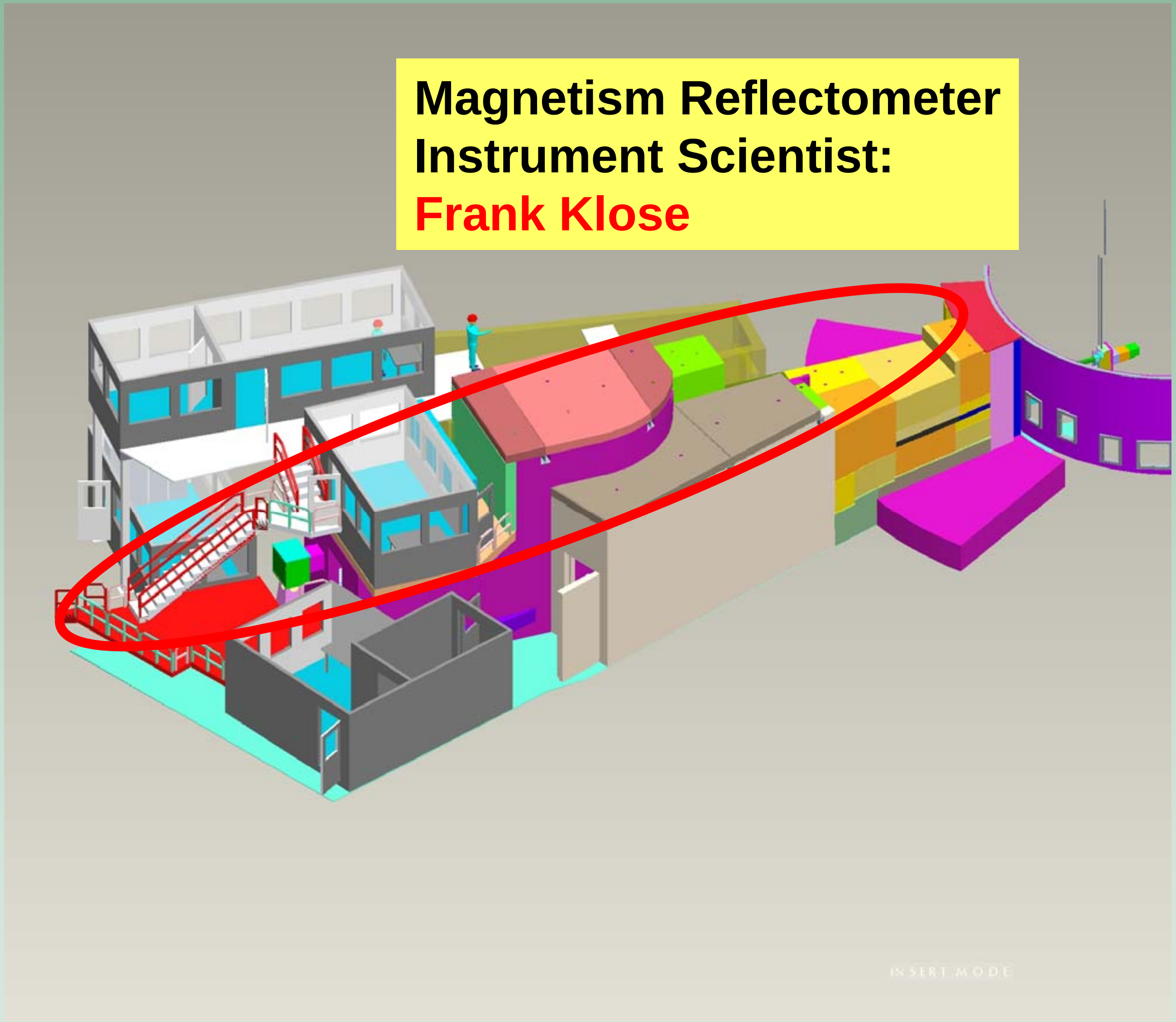
4: off-specular diffraction (below horizon)

$$\theta = \theta_i + \sqrt{\theta_i^2 + 2n\lambda / d - Nb\lambda^2 / \pi} \quad \text{with } n = -1$$

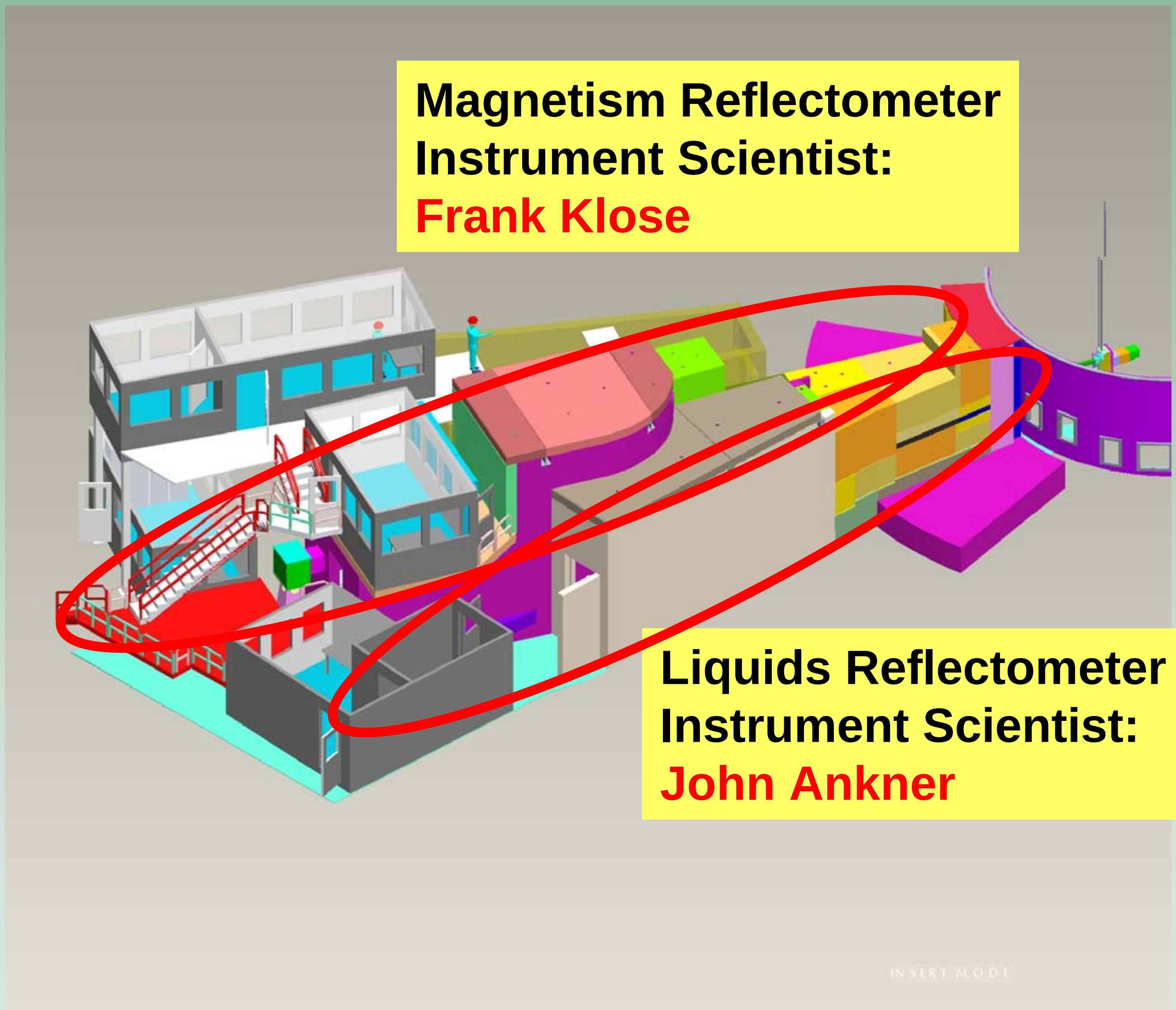
(dashed lines are the critical edges: from the horizon to higher/lower angles, the silicon edge -above the horizon only- and the permalloy edges)

W.T. Lee, F. Klose, H.Q. Yin, B.P. Toperverg, Physica B 335 (2003) 77–81

SNS Reflectometers



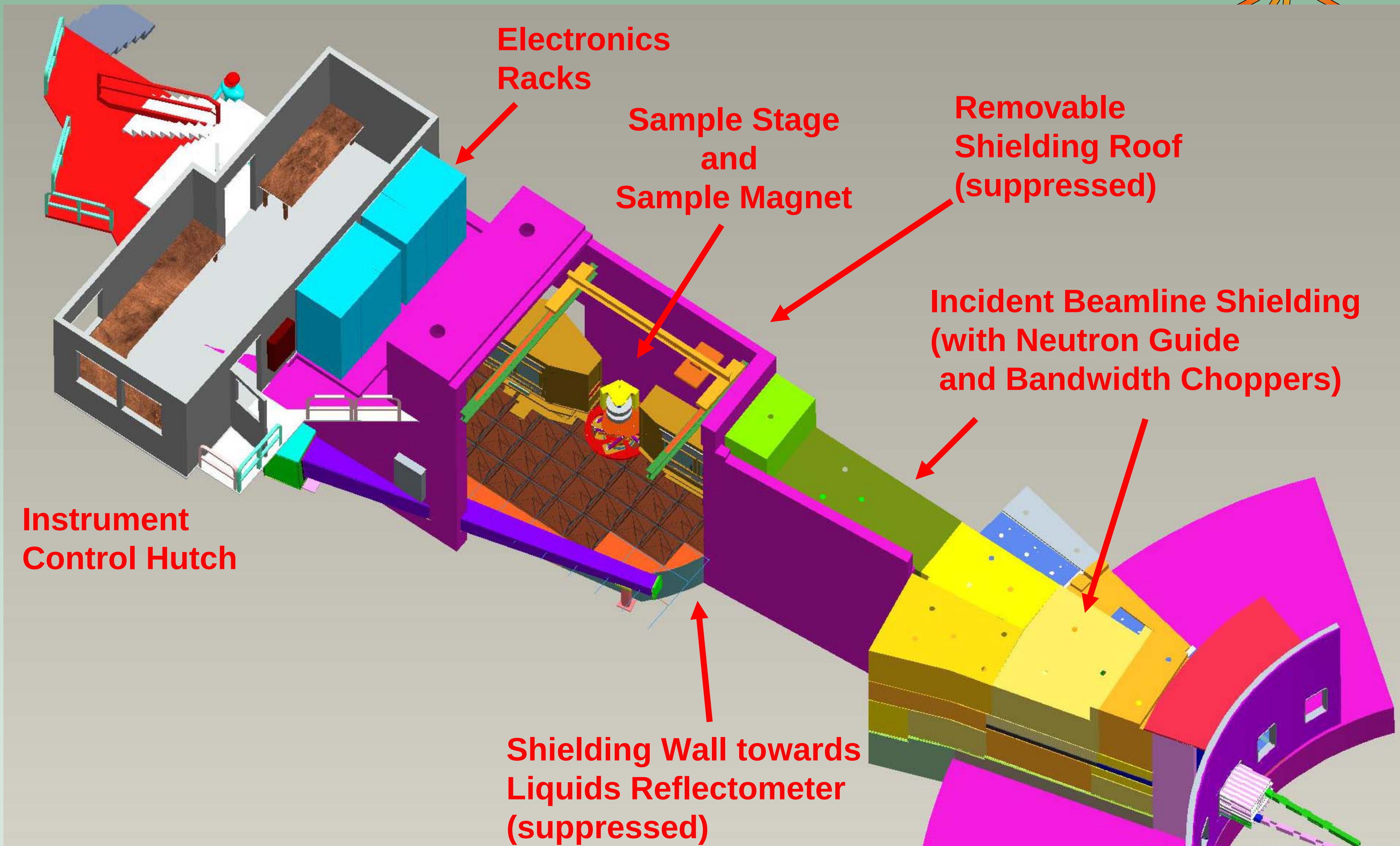
SNS Reflectometers



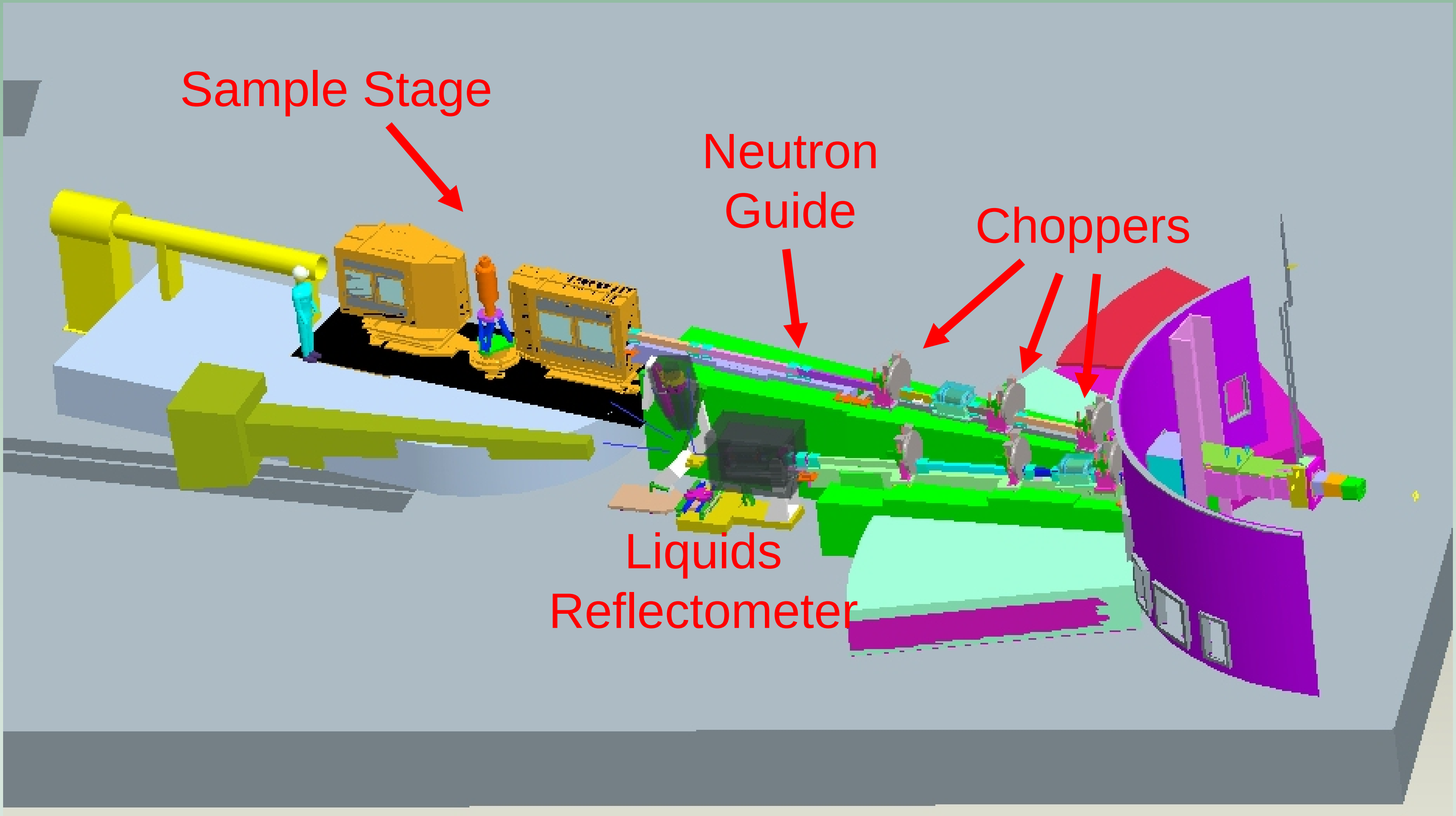
Instrument Enclosure Construction

Magnetism Reflectometer - Overview

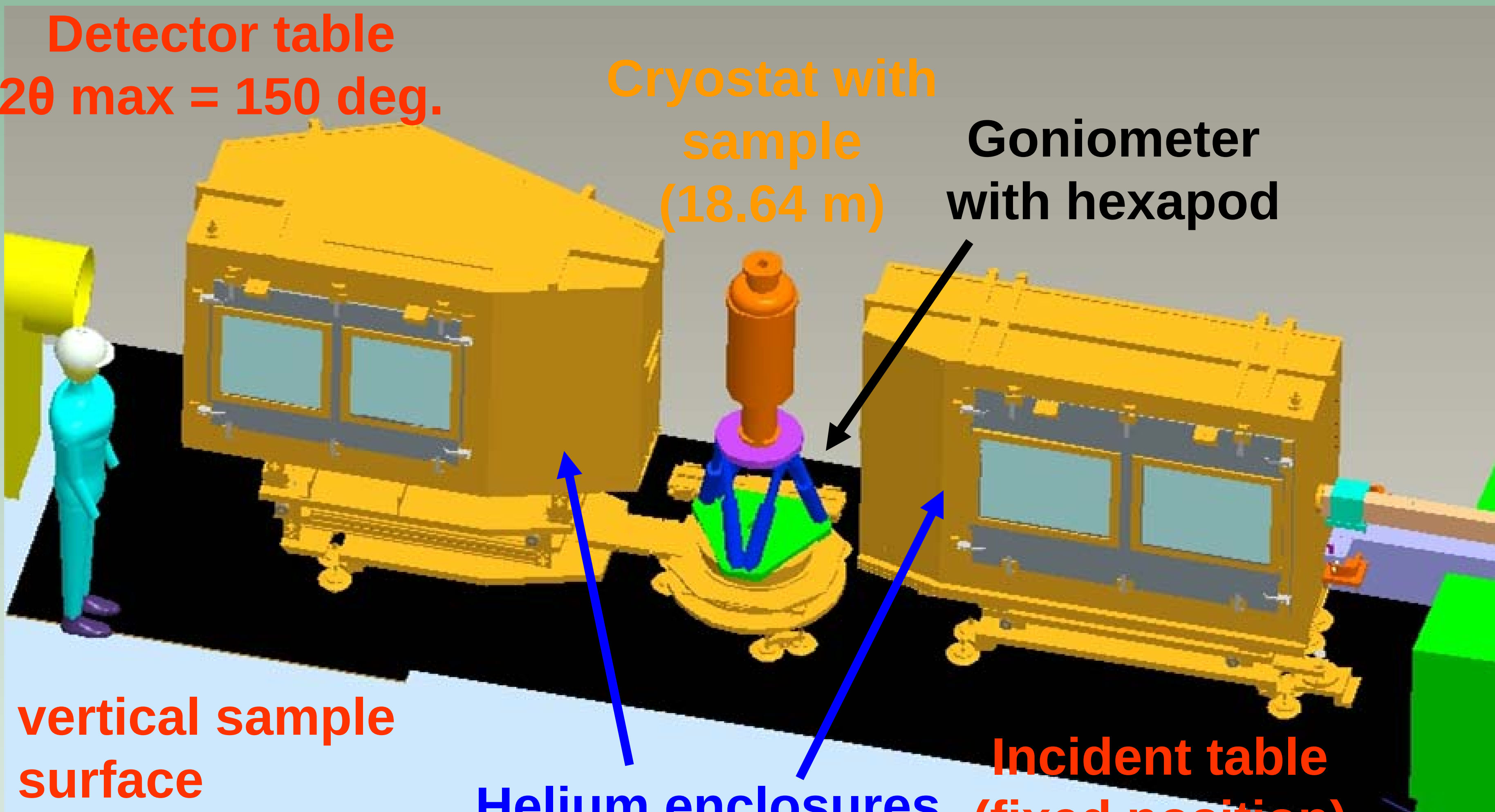
SPALLATION NEUTRON SOURCE



Magnetism Reflectometer - Overview

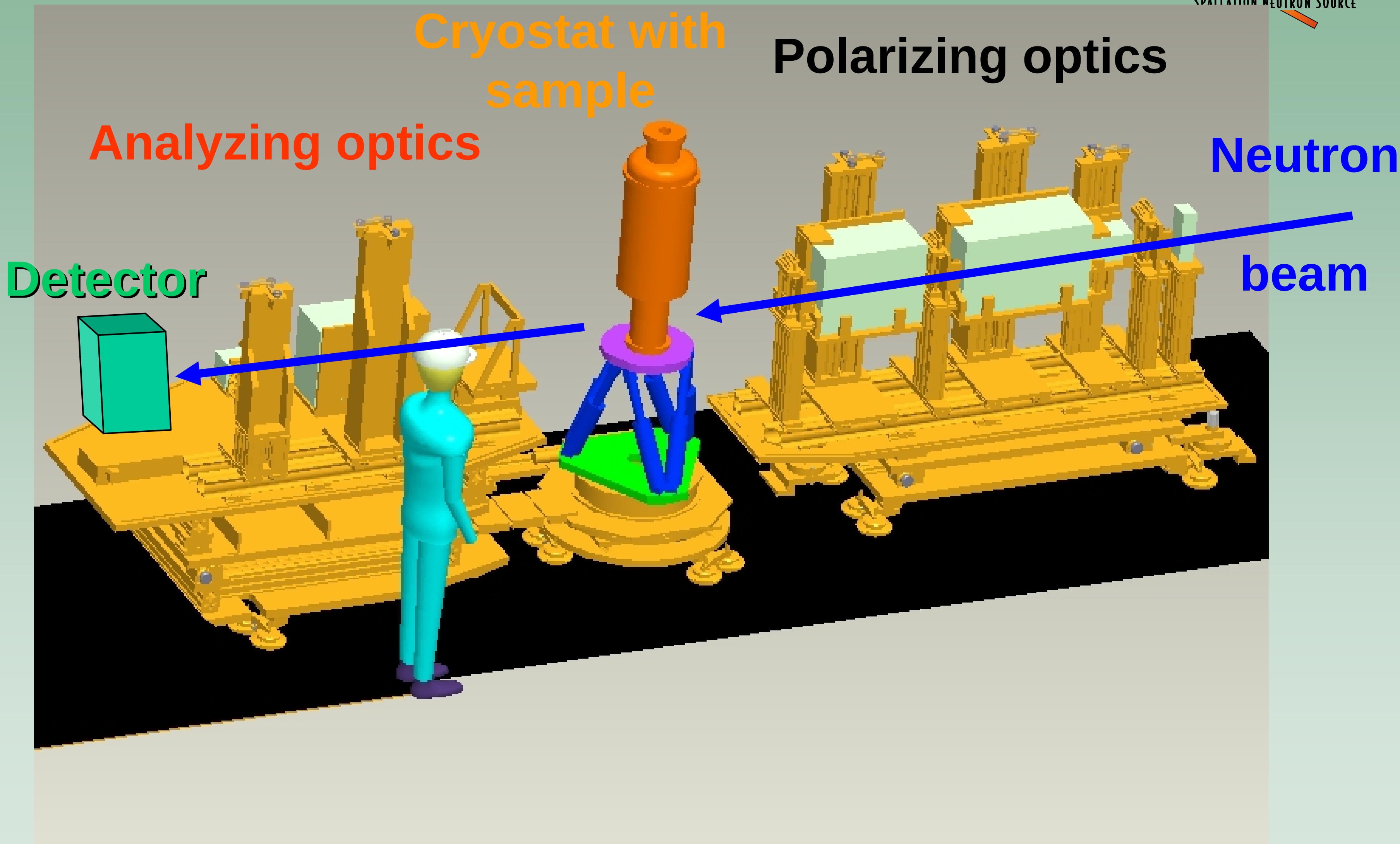


Sample Stage



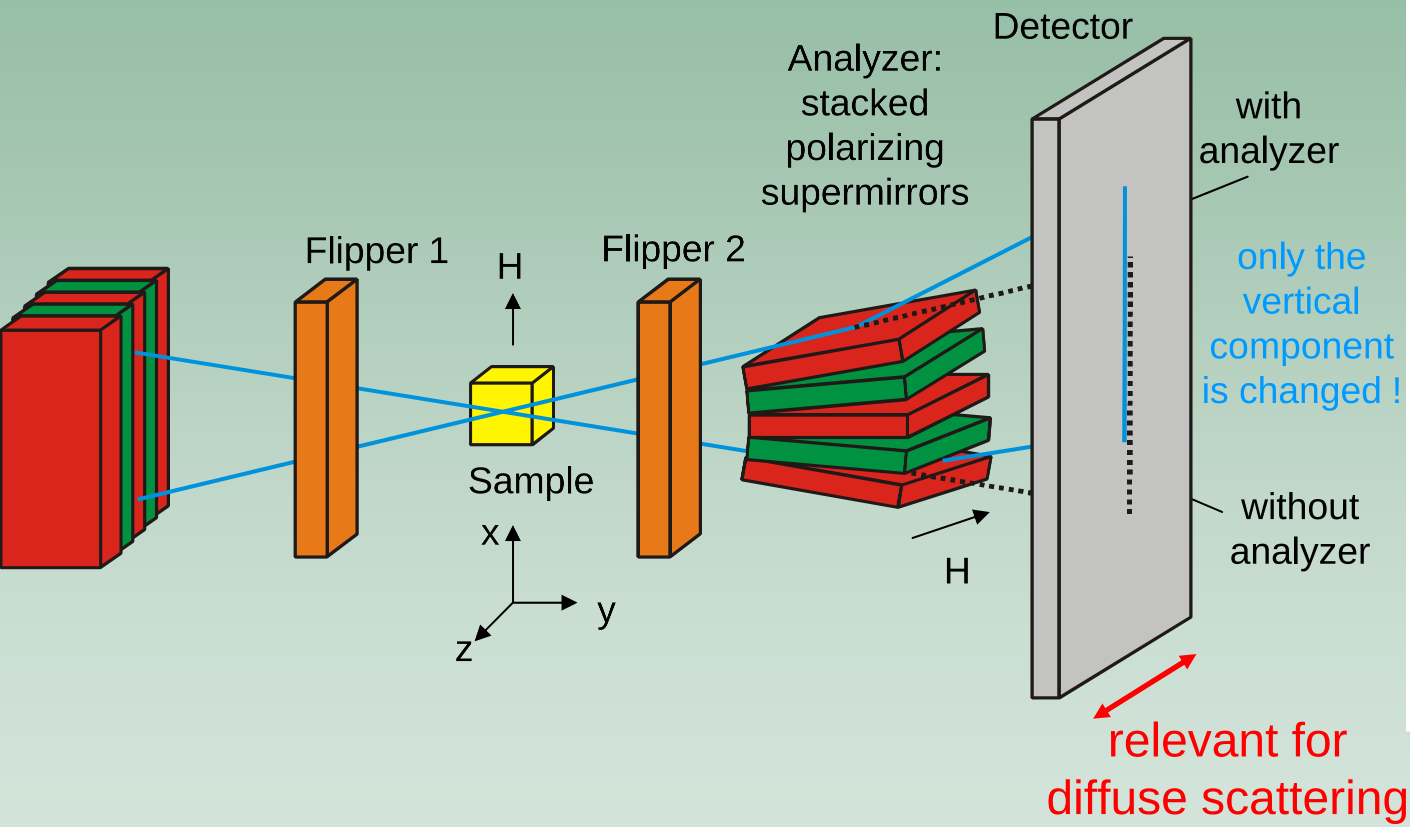
Q_{max} ~ 7 Å^{-1}

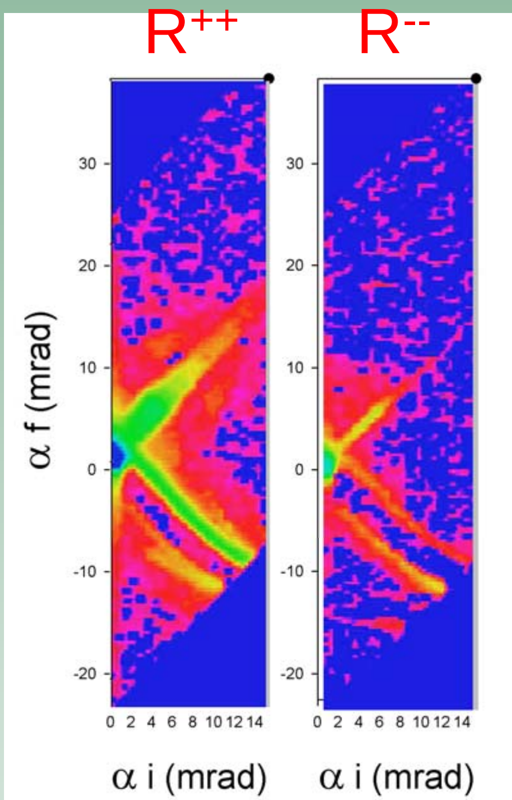
Sample Stage



Assembly of Sample Stage

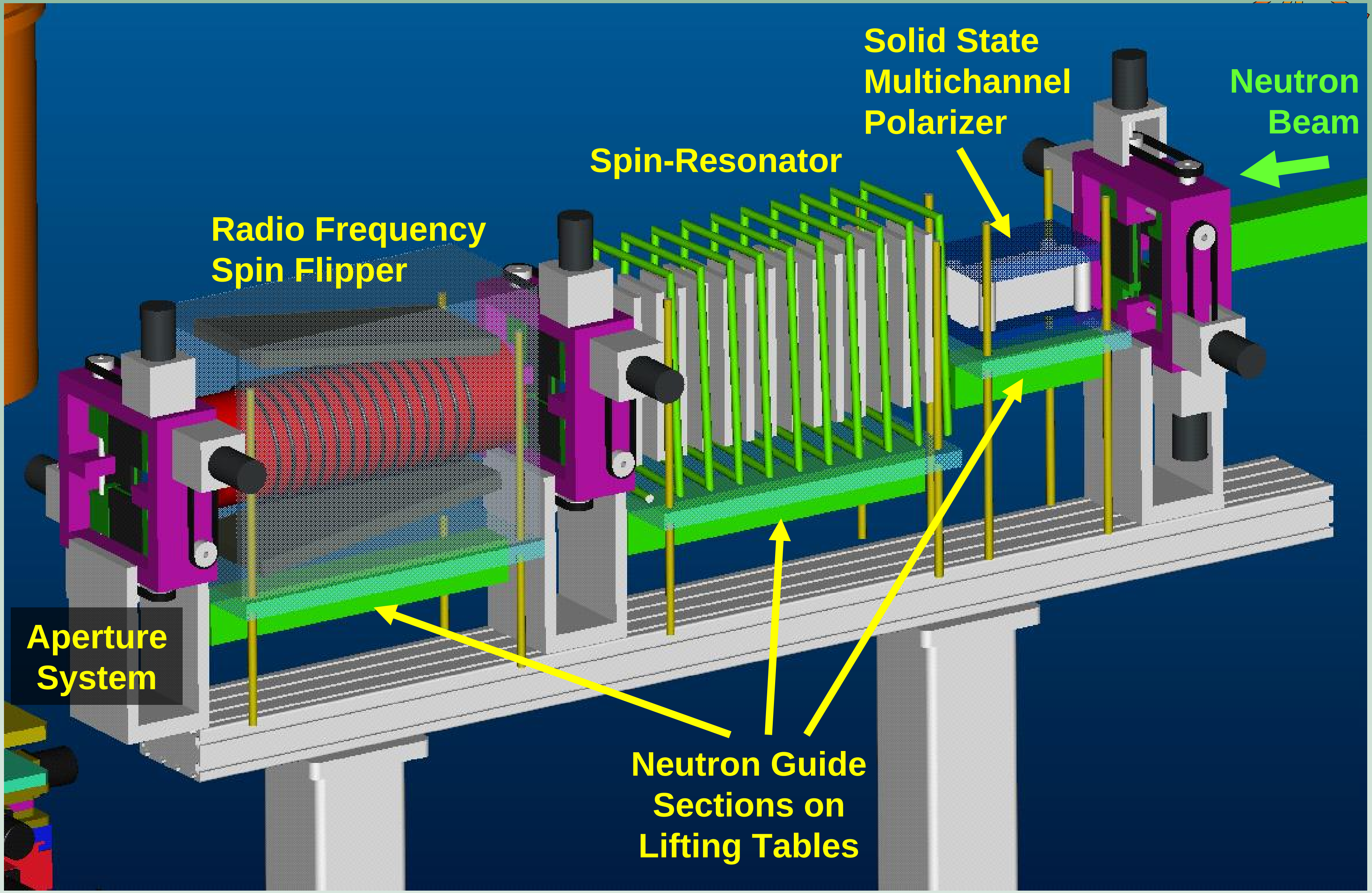
Polarized Neutron Off-Specular Scattering with Polarization Analysis



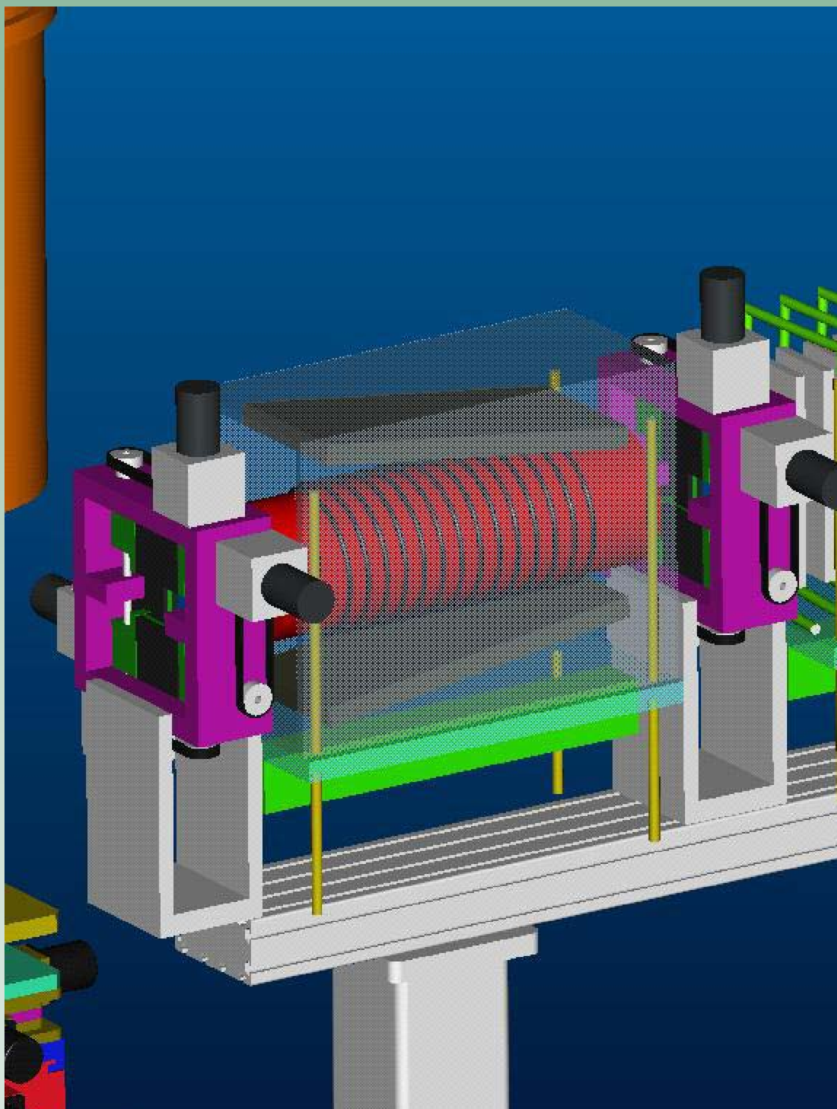


W.T. Lee, F. Klose, B. Toperverg, U. Ruecker
measured at HADAS reflectometer, FZ Juelich, Sept. 2002

Polarized Beam Devices



Spin Flipper (SNS Design - A. Parizzi)



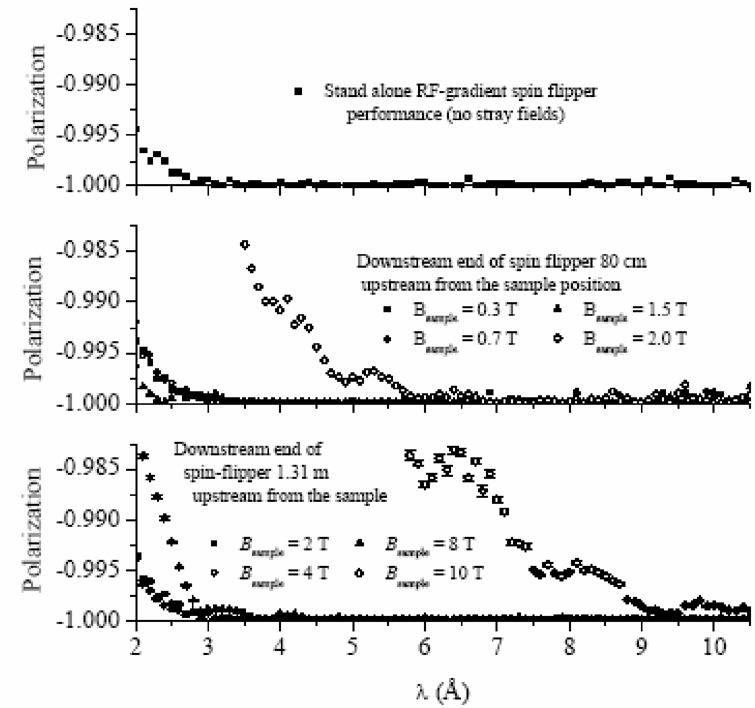


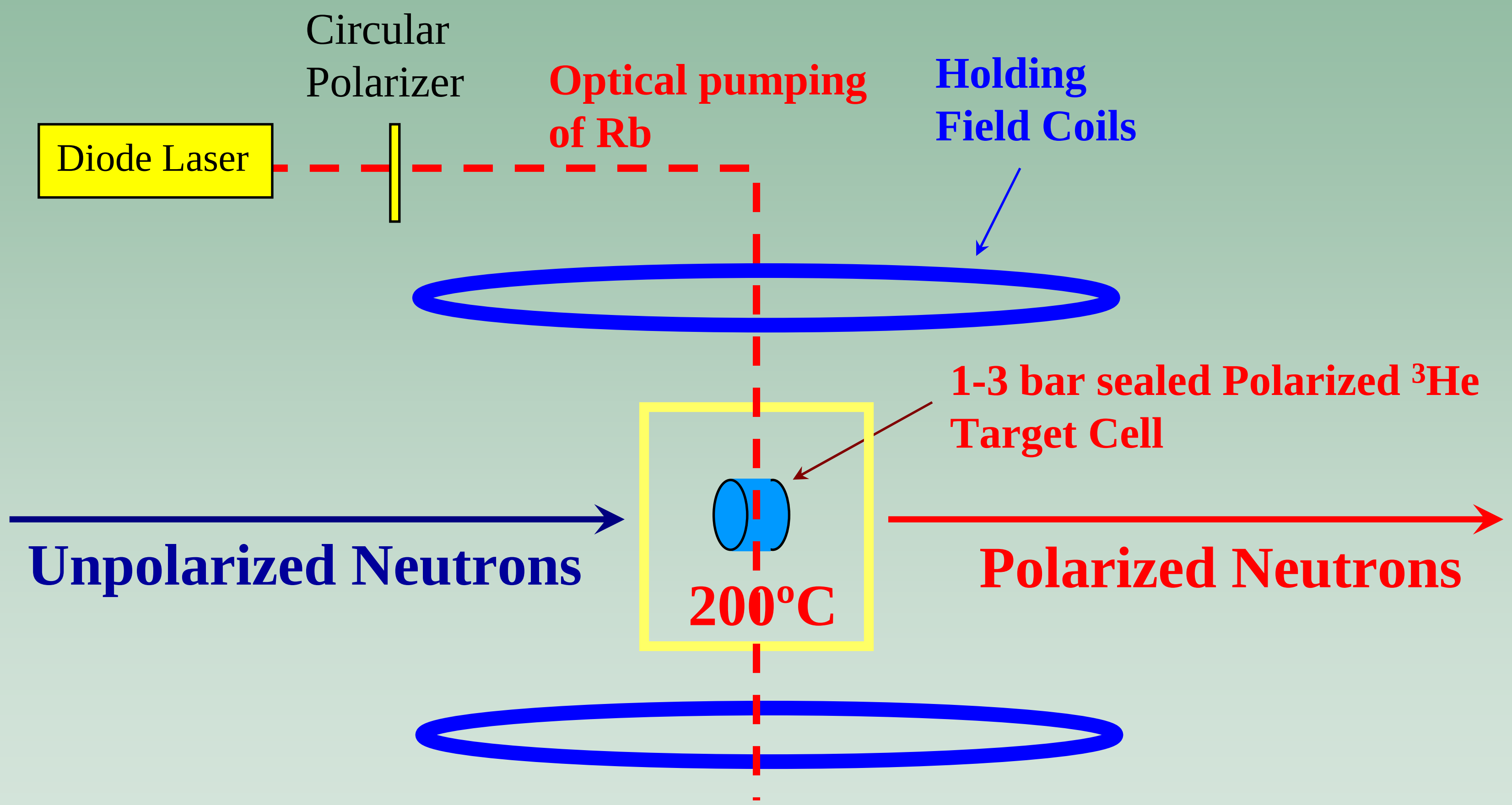
Figure 2 – Calculated performance of the RF-gradient flippers for the Magnetism Reflectometer for various sample magnetic flux densities and distances to the magnet.

Neutron polarization evolution calculations along the SNS Magnetism Reflectometer beam line

André de A. Parizzi, Frank Klose Volker Christoph

PNCMI 2004 Proceedings

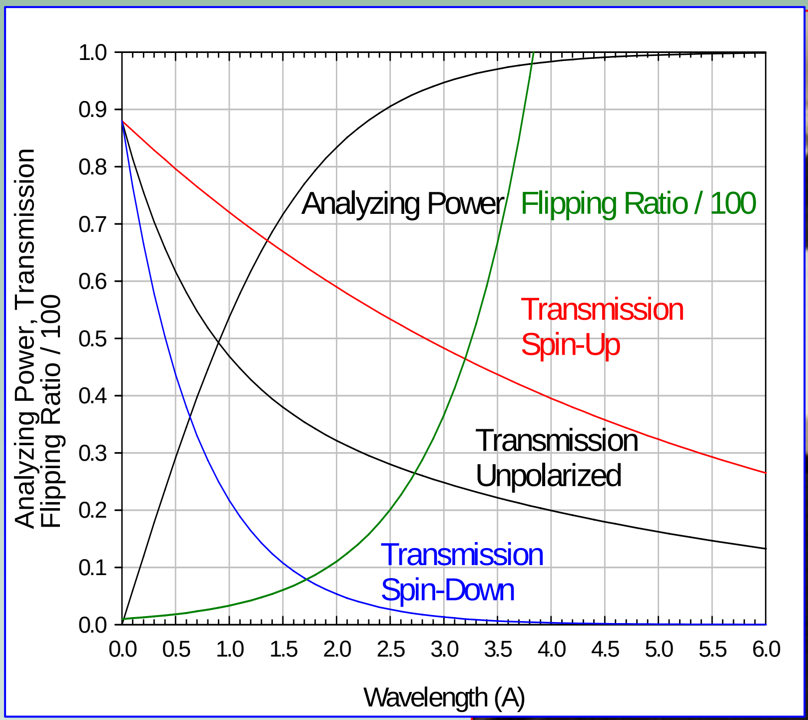
^{3}He Analyzer System (courtesy: Hal Lee)

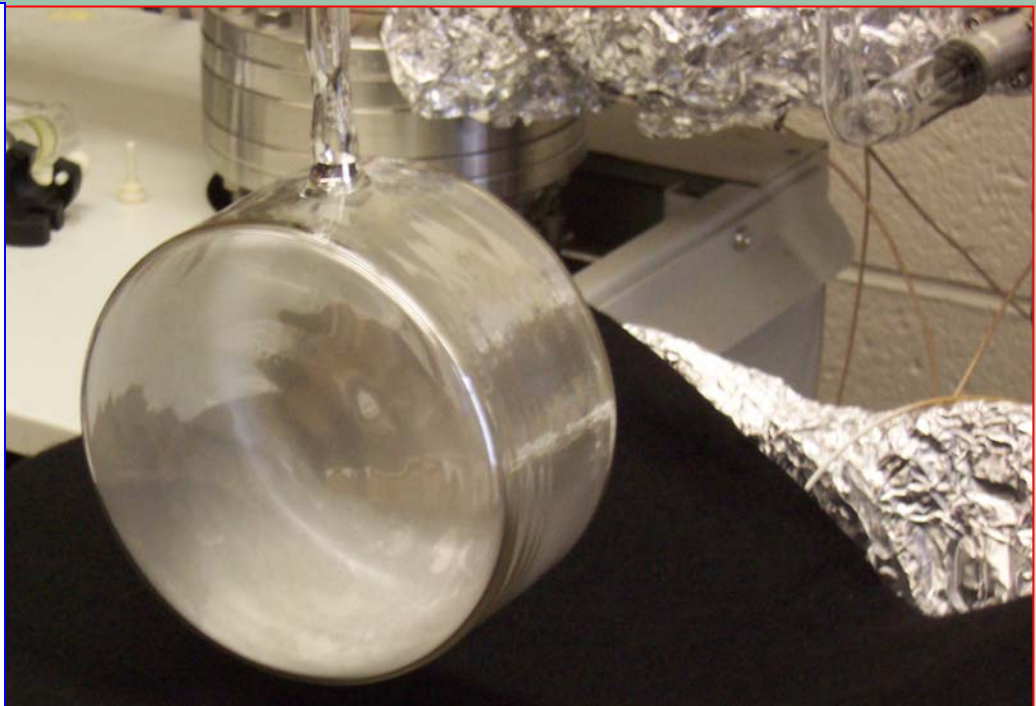


Rb atom transfers its polarization to ^{3}He by collision. Then ^{3}He nuclei is polarized by hyperfine interaction.

^{3}He Analyzer System (courtesy: Hal Lee)

- **Procurement of parts is underway.**
- **^{3}He cell filled (photo below).**
- **Test completed system on neutron beam in October/November.**





- **Diameter = 12 cm, Length = 7.5 cm (inner dimensions)**
- **3He pressure 1.5 bar**
- **Effective for 2-5 Å neutrons**

The Magnetism Reflectometer Team

- Frank Klose - Instrument Scientist Magnetism Reflectometer
- Tim Chae - Lead Engineer (SNS)
- Roger Kellogg - Engineer (ANL)
- Andre Parizzi - Electrical Engineer (Polarized Neutrons)
- Hal Lee - Polarized Neutron Scientist (^{3}He Analyzer)
- Richard Goyette - Scientific Associate
- John Ankner - Liquids Reflectometer