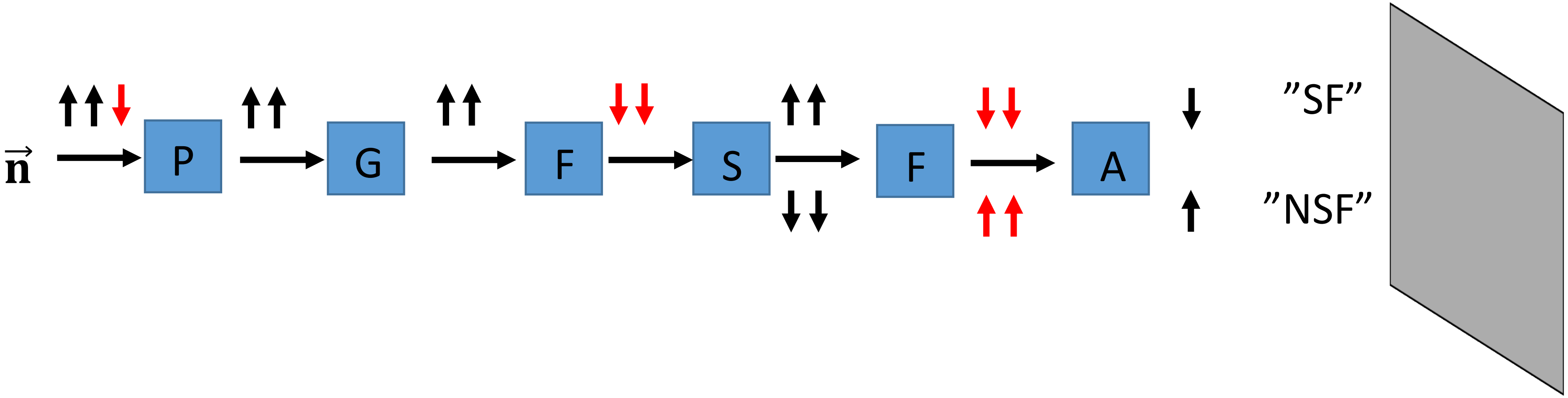
Overview on data correction for polarized SANS

(1) Overview ^{3}He-cells and Supermirrors

(2) Data reduction steps
   (a) ^{3}He + ^{3}He (DREAM)
      - DB measurements with 2 channels on both cells
   (b) SM + ^{3}He (SKADI)
      - DB measurements with 4 channels
      - DB measurements with 2 channels

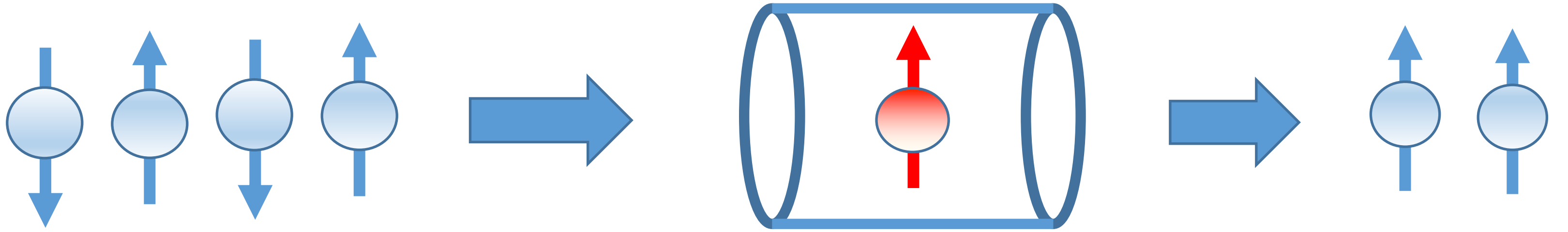
(i) Neutron polarizers and analyzers



(1) How are neutrons polarized?
→ Polarizer, "P"
(2) How are they transported?
→ Guide field, "G"
How are they flipped?
→ Flipper, "F"
How is the neutron polarization read out?
→ Analyzer, "A"

(i) Neutron polarizers and analyzers: ^{3}He glass cells

Based on spin-dependent neutron absorption cross-section of ^{3}He



$n + {}^3He \rightarrow {}^3H + {}^1H + 764$ keV

<u>^{3}He-cell:</u>

- Filled with polarized ^{3}He atoms
- Transmission of neutrons with $\mathbf{s}_n \mathbin{||} \mathbf{s}_{He}$
  - ➢ σ++ ≈ 5 barn
- Adsorption of neutrons with $\mathbf{s}_n \mathbin{||} -\mathbf{s}_{He}$
  - ➢ σ+- ≈ 6000 barn
- Reversal of $\mathbf{s}_{He}$ by NMR-pulses
- **Atomic polarization of ^{3}He-atoms decays with time!**

$$P(3He)(t) = \tanh(\mu * AP(t))$$

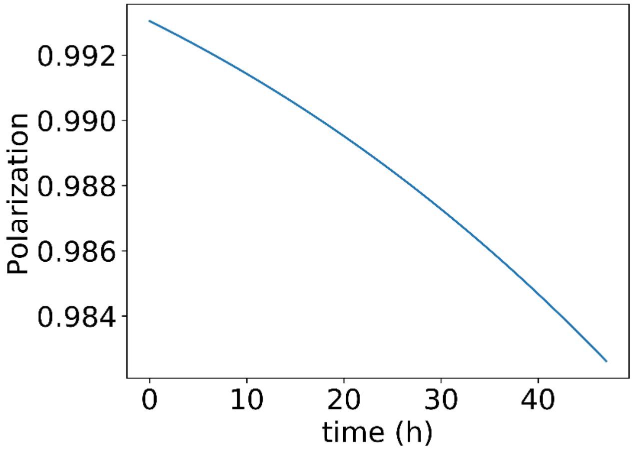
AP(t)
= Atomic polarization
= $AP = AP_0 * \exp(-\Delta t/\gamma)$

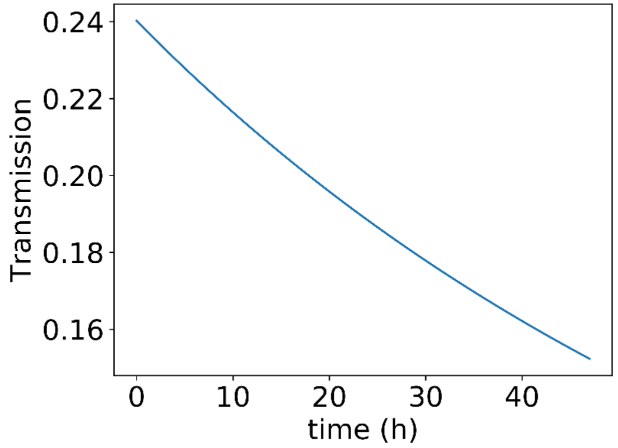
μ= opacity of ^{3}He-cell

$$T({}^3He)(t) = \mathrm{TE} * \exp(-\mu) * \cosh(\mu * AP(t))$$

TE = transmission of unfilled cell

γ = decay time constant



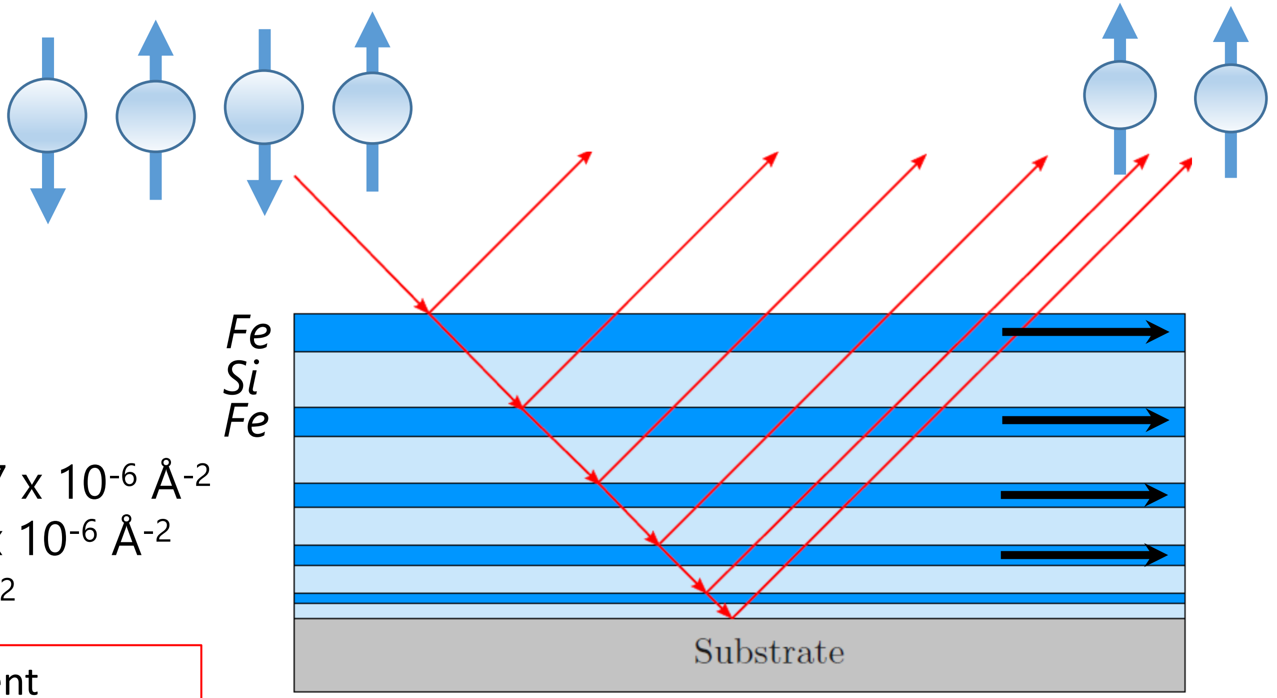


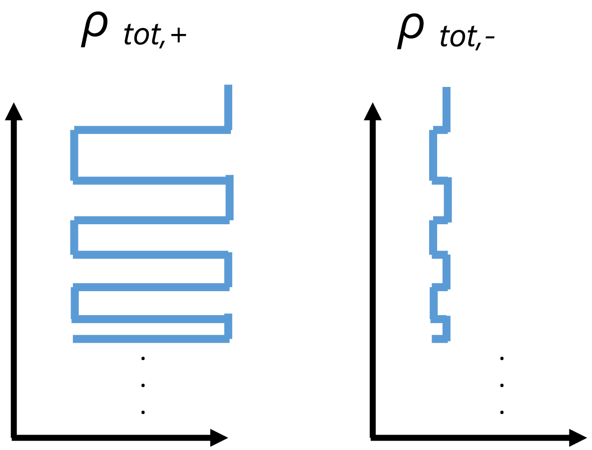
Correction of measurements

$$\boldsymbol{I = I(measured)(t)/Trans(t)}$$

[1] K. Krycka et al., *Physica B* **404,** 2561-2564 (2009).
[2] R. P. Hermann, *Neutron Scattering Lectures*, Forschungszentrum Jülich GmbH (2015), vol. 106

(i) Neutron polarizers and analyzers: Supermirrors





$\rho_{tot} = \rho_n \pm \rho_m$

$\rho(Fe, Spin+) = 12.97 \times 10^{-6}$ Å^{-2}

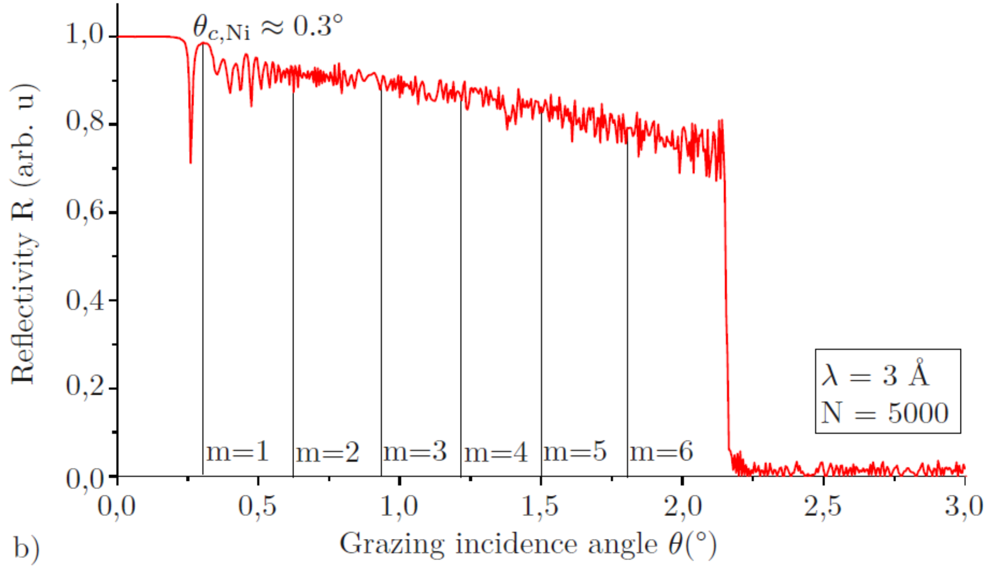
$\rho(Fe, Spin-) = 3.08 \times 10^{-6}$ Å^{-2}

$\rho(Si) = 2.08 \times 10^{-6}$ Å^{-2}

Based on spin-dependent neutron scattering length of magnetized Fe layers!

Supermirror:

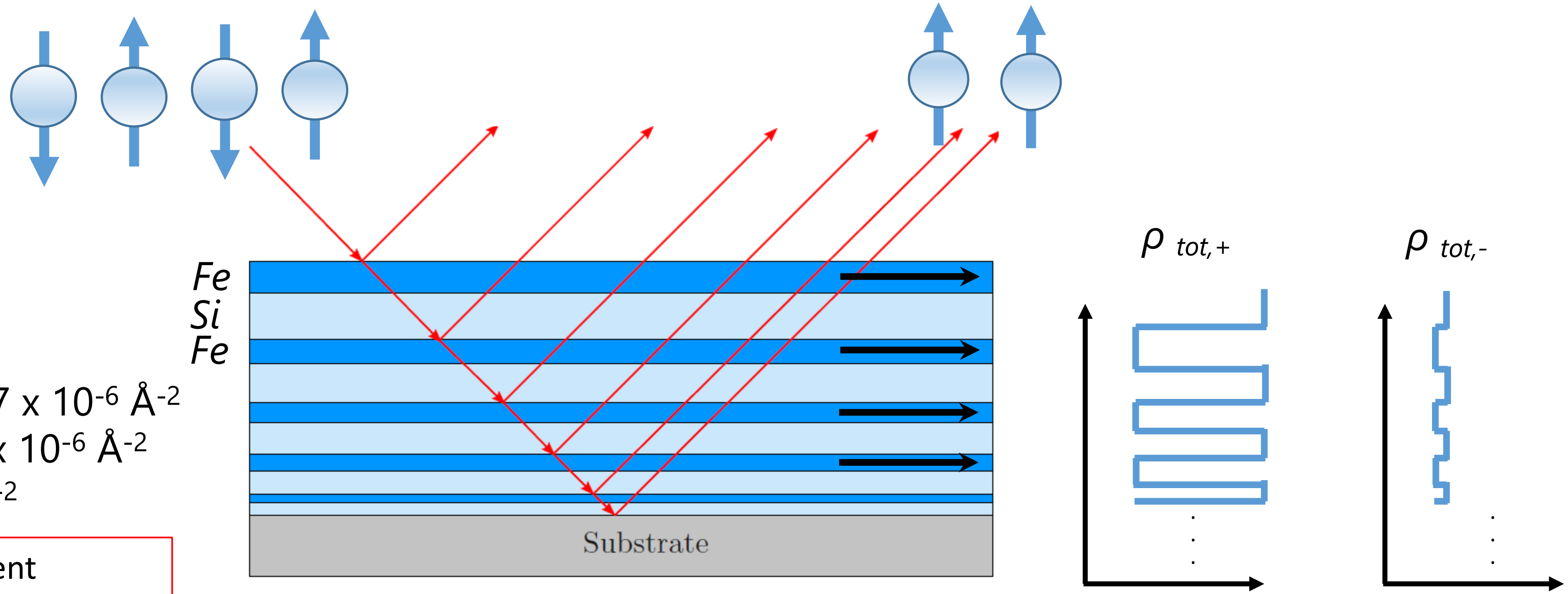
- FeSi multilayers
- High reflectivity for one spin state, high transmission for other
- Broad total reflection niveau due to multiple Bragg angles
- „m-value“ ≈ number of layers ≈ $\theta_{tot,max}$



b)

[1] S. Broekhuijsen, PhD thesis, University of Linköping (2021).

(i) Neutron polarizers and analyzers: Supermirrors



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Based on spin-dependent neutron scattering length of magnetized Fe layers!

➢ **Critical: interface roughness**

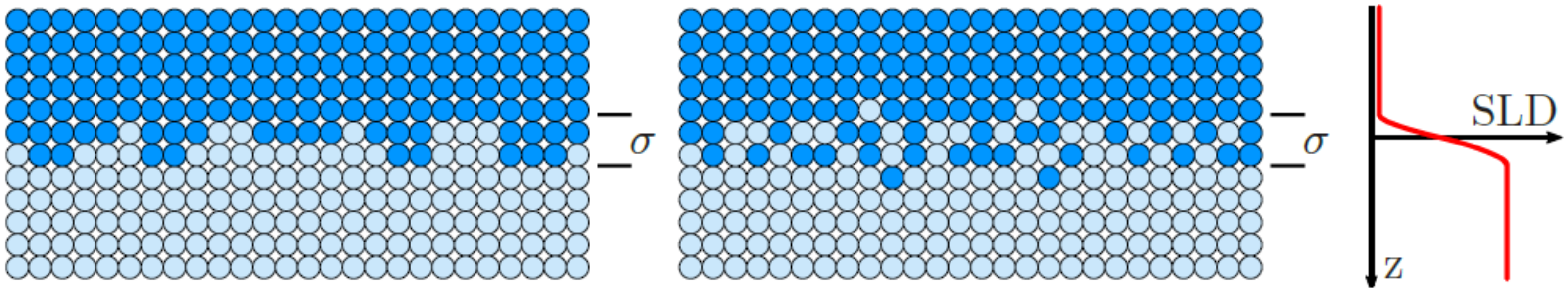
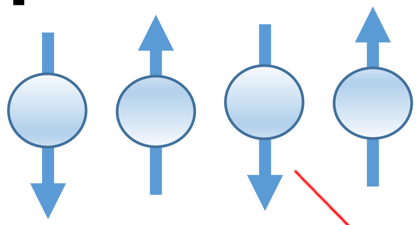
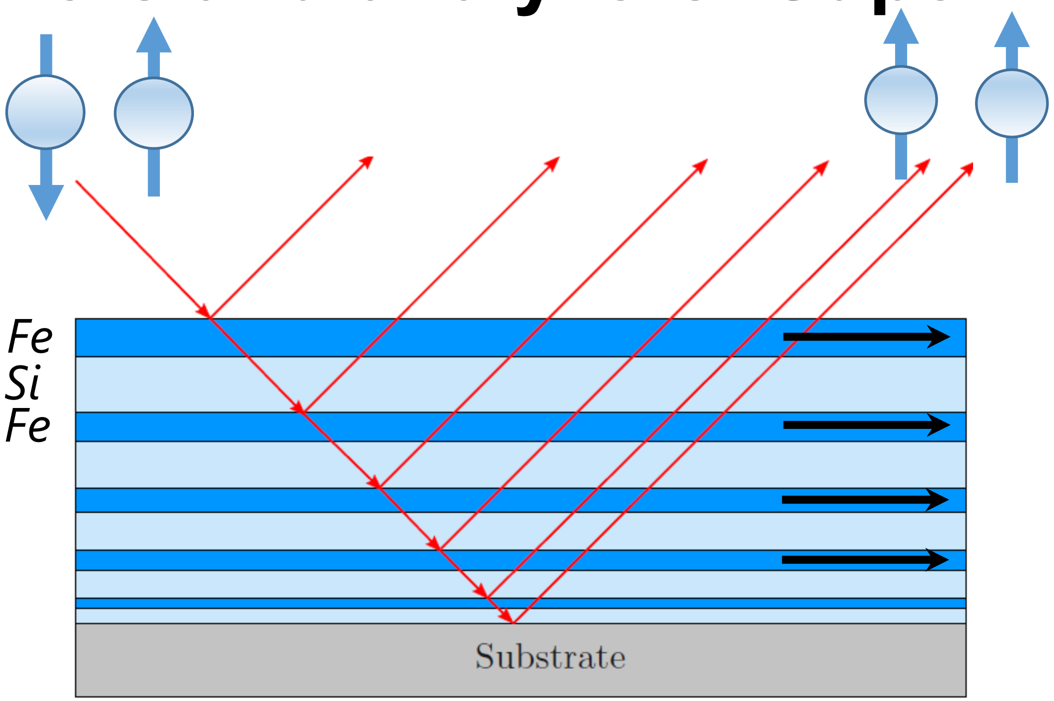


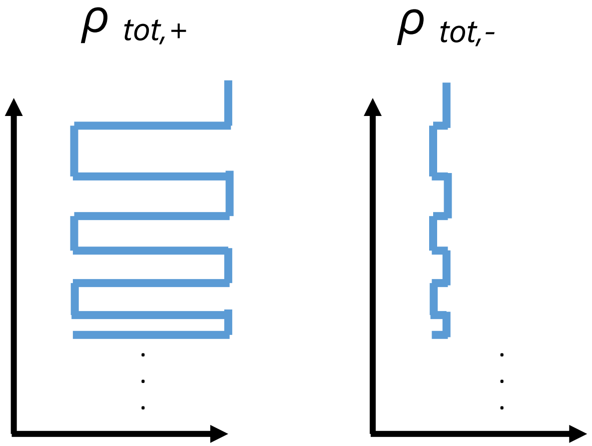
Figure 3.7: While intermixing and surface roughness are distinct phenomena, they are indistinguishable in the SLD profile normal to the interface.

[1] S. Broekhuijsen, PhD thesis, University of Linköping (2021).

(i) Neutron polarizers and analyzers: Supermirrors







$\rho_{tot} = \rho_n \pm \rho_m$

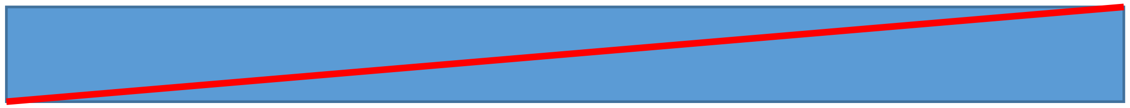
$\rho(Fe, Spin+) = 12.97 \times 10^{-6}$ Å^{-2}

$\rho(Fe, Spin-) = 3.08 \times 10^{-6}$ Å^{-2}

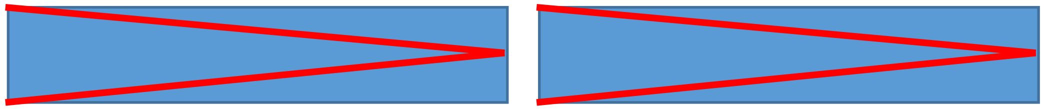
$\rho(Si) = 2.08 \times 10^{-6}$ Å^{-2}

Different geometries:

Single mirror

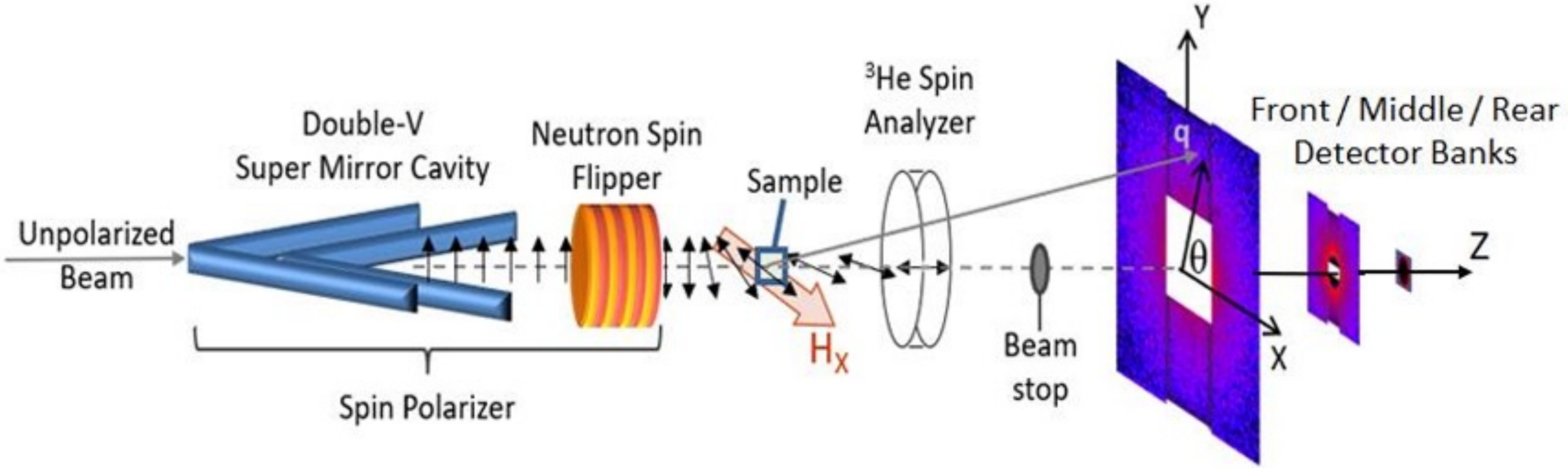


V-cavity



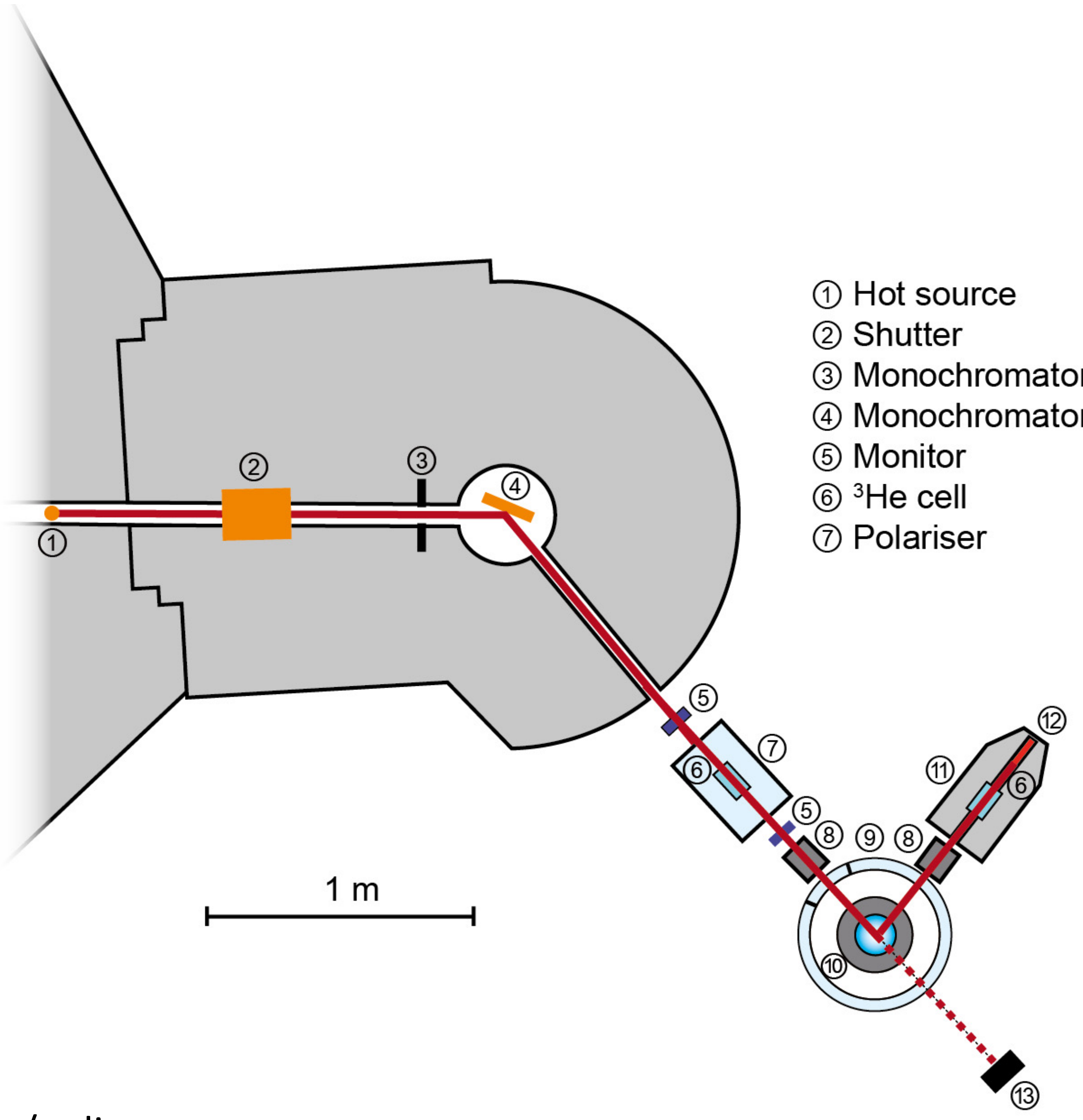
In courtesy of W. T. Hal Lee

(ii) Example setup: Pol-SANS (SM + 3He)



https://www.nist.gov/ncnr

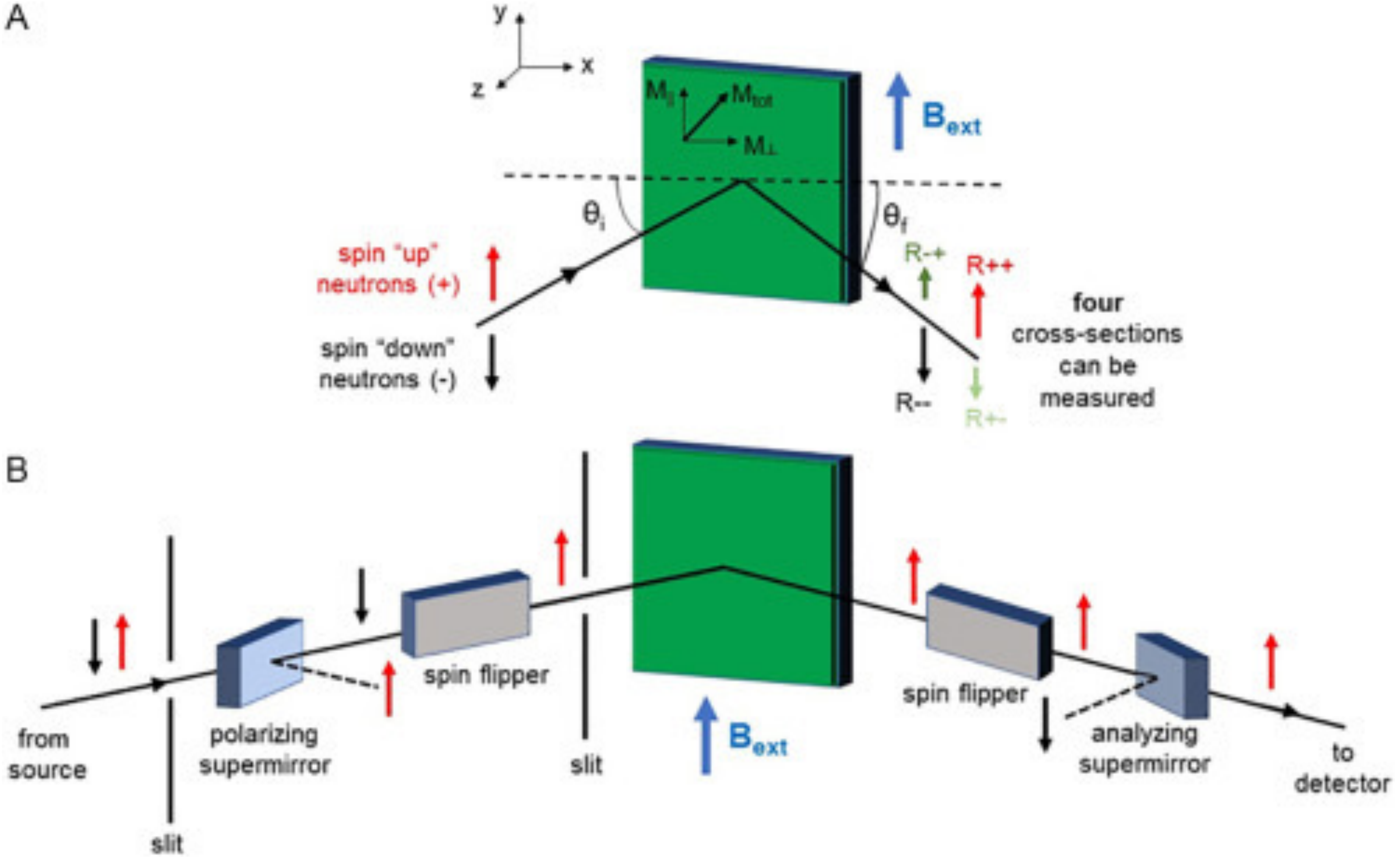
(ii) Example setup: PND (3He + 3He)



① Hot source
② Shutter
③ Monochromator slits
④ Monochromator
⑤ Monitor
⑥ ^{3}He cell
⑦ Polariser
⑧ Nutator
⑨ Cryopad/ Cryomagnet
⑩ Cryostat with sample
⑪ Analyser
⑫ Detector
⑬ Beam stop

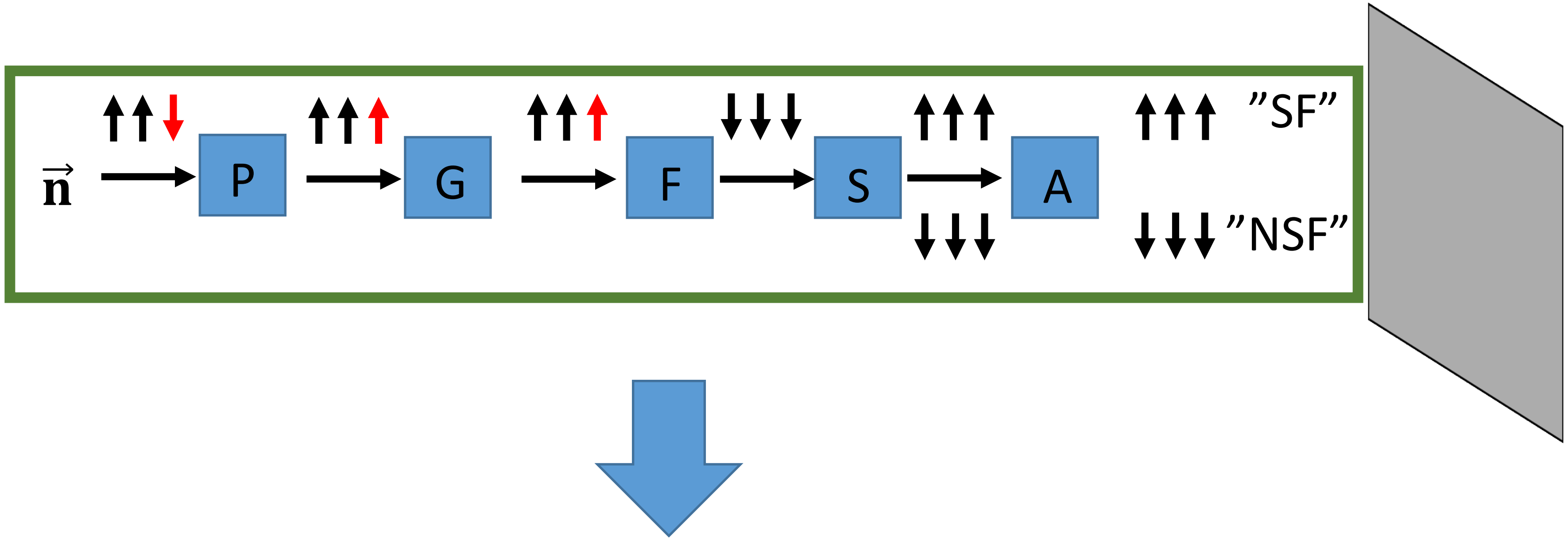
https://mlz-garching.de/poli

(vi) Example setup: PNR (SM + SM)



S. J. Callori et al., https://doi.org/10.1016/bs.ssp.2020.09.002

(iii) Data analysis under consideration of all components



Effect on measured intensities?

$$\begin{pmatrix} I_{++} \\ I_{+-} \\ I_{-+} \\ I_{--} \end{pmatrix} \sim \frac{d\boldsymbol{\sigma}}{d\Omega} = \begin{pmatrix} S_{++} \\ S_{+-} \\ S_{-+} \\ S_{--} \end{pmatrix}$$

(iii) Data analysis under consideration of all components

$$I \sim \frac{d\sigma}{d\Omega} = \begin{pmatrix} S_{++} \\ S_{+-} \\ S_{-+} \\ S_{--} \end{pmatrix} \qquad \begin{pmatrix} \mathrm{I}_{++} \\ \mathrm{I}_{+-} \\ \mathrm{I}_{-+} \\ \mathrm{I}_{--} \end{pmatrix} = \mathrm{I}_0 \cdot \begin{pmatrix} A_+ & A_- & & \\ A_- & \mathrm{A}+ & & 0 \\ & 0 & A_+ & A_- \\ & & A_- & A_+ \end{pmatrix} \cdot \mathbf{F2} \cdot \mathbf{F1} \cdot \begin{pmatrix} P_+ & 0 & P_- & 0 \\ 0 & P_+ & 0 & P_- \\ P_- & 0 & P_+ & 0 \\ 0 & P_- & 0 & P_+ \end{pmatrix} \cdot \begin{pmatrix} \mathrm{S}_{++} \\ \mathrm{S}_{+-} \\ \mathrm{S}_{-+} \\ \mathrm{S}_{--} \end{pmatrix}$$

I =measured intensities
S = The sample's scattering cross-section → what we want to get from the data reduction.
P = Polariser spin-dependent transmission matrix
A = Analyser spin-dependent transmission matrix
F1, F2 = spin-flipper matrices, if present → If they work with 100% efficiency: ***F1, F2*** = ***1 (identity matrix)***

[P, A] = 0 → P & A commute, order does not matter
[P, F] ≠ 0 → the matrices must be in order!

[1] W.T. *Lee et al.*, "Polarisation Development at the European Spallation Source", EPJ Web of Conferences **286**, 03004 (2023)

Background information on 3He-cell transmission correction

Definitions:

Nuclear polarization of 3He cell	$P_{He}(t)$	→ same for +/- states, λ -independent
Opacity of ^{3}He-cell:	O(λ)	→ same for +/- states, λ -dependent
Transmission empty 3He glass:	TE	→ same for +/- states, λ -independent
Transmission unpolarized neutron beam:	$Transmission^{unpol}(t,\lambda)$	→ same for +/- states, λ -dependent

Corrections to be done for each He cell:

1. Opacity + unpolarized cell tranmission

(a) Either by measurement of pressure from ^{3}He-team after filling:

$$O(\lambda) = 0.0733\, p\, l\, \lambda$$

(b) Or by neutron beam:

$$O(\lambda) = -ln\left[\frac{I^{unpol.beam}_{unpolarized\ ^3He\ cell} - I_{bg,\ He}}{I^{unpol.beam}_{^3He\ cell\ out} - I_{bg,\ noHe}} \frac{1}{TE}\right)]$$

2. Initial nuclear polarization

$$P_{He0}(t_0) = acosh\left[\frac{I^{unpol.beam}_{polarized\ 3He\ cell} - I_{bg,\ He}}{I^{unpol.beam}_{^3He\ cell\ out} - I_{bg,\ noHe}} \frac{1}{TE \cdot exp(O(\lambda))}\right]/O(\lambda)$$

3. Time-decay

$$P_{He}(t) = \mathrm{P}_{\mathrm{He0}}(t_0) * \exp(-\frac{\Delta t}{T_1})$$

Details are listed for each step on the next slides

4. Determine correction factors for polarization dependent cell transmission

$$Transmission^{\pm}(t,\lambda) = \mathrm{TE} * \exp(-O(\lambda) \pm O(\lambda) * P_{He}(t))$$

Detailed Data-correction procedure

1. Opacity + unpolarized cell tranmission

There are 2 ways to measure the opacity:

(a) By measurement of pressure from ^{3}He-team after filling

$O(\lambda)$= 0.0733 $p\ l\ \lambda$

- disadvantage: measurement of p not very precise
- advantage: Can work as a fast first estimation without measurement of the unpolarized cell

Fix input values	Cell pressure, p	Cell length, l	Wavelength, λ
Neutron data input	None		
Parameters to compute	Opacity O (λ)		

(b) By neutron beam measurements:

$$O(\lambda) = -ln[\frac{I^{unpol}_{unpolarized\ ^3He\ cell} - I_{bg,\ He}}{I^{unpol}_{^3He\ cell\ out} - I_{bg,\ noHe}} \frac{1}{TE)}]$$

- advantage: more accurate
- disadvantage: cell needs to be depolarized, i.e., would be done only at the end of its lifetime (i.e., after ca. 1 day)

→ (b) Should be done at the end of the day/experiment for very precise data reduction

→ (a) should be taken in the beginning for live-data reduction, but afterwards being overwritten by (b)

Fix input values	Transmission empty glass, TE	Wavelength, λ
Neutron data input	DB transmission of - unpolarized neutron beam - unpolarized 3He cell $I^{unpol}_{unpolarized\ 3He\ cell}$	DB Transmission of - unpolarized neutron beam - no cell in (moved out) $I^{unpol}_{^3He\ cell\ out}$
Parameters to compute	Opacity O (λ)	

Detailed Data-correction procedure

2. Initial nuclear polarization

Step Nr. 2 : Determination of time-independent prefactor of the 3He-cell time decay:

$$P_{He0} = acosh\left[\frac{I^{+\,or\,-}_{polarized\ ^3He\ cell} - I_{bg,\,He}}{I^{unpol}_{^3He\ cell\ out} - I_{bg,\,noHe}} \frac{1}{TE \cdot exp(O(\lambda))}\right]/O(\lambda)$$

To note:

(1) $P_{He0}(t_0)$ is polarization independent

- Up/ Down polarized cells would give same result for the direct beam measurement: $I^{+}_{polarized\ 3He\ cell}$ = $I^{-}_{polarized\ 3He\ cell}$
- Take only one polarization direction for the calculations (saving time)

(2) T_{bg} is to be taken from the same measurement as T, but far away from Direct Beam region

- probably need some maskfile
- this is important in case the background with 3He cell is different than without 3He cell

Fix input values	Transmission empty glass, TE	Opacity, $O(\lambda)$
Neutron data input	DB transmission of - half-polarized neutron beam - polarized 3He cell (any pol.-direction) - according background data I^+ or I^-	DB Transmission of - unpolarized neutron beam - no cell in (moved out) - according background data $I^{unpol}_{^3He\ cell\ out}$
Parameters to compute	Nuclear polarization at time t0, $P_{He0}(t_0)$	

Detailed Data-correction procedure

3. Time-decay of nuclear polarization:

Step Nr. 3 : Determination of time-dependency of each 3He-cell:

$$P_{He}(t_n) = \mathrm{P}_{\mathrm{He0}} * \exp(-\frac{t_0 - t_n}{T_1})$$

To note:

(1) $P_{He}(t)$ is polarization independent

- Up/ Down polarized cells would give same result
- Take only one polarization direction for the calculations (saving time)

(2) T_{bg} is to be taken from the same measurement as T, but far away from Direct Beam region

- probably need some maskfile
- this is important in case the background with 3He cell is different than without 3He cell

Fix input values	Start time of using ^3He cell in the beamline (start of first measurement), t_0	Time stamp t_n
Neutron data input	DB transmission of - unpolarized neutron beam - polarized 3He cell (P+A) (any pol.-direction) - take this as function of time! I^+ or I^-	
Parameters to compute	Nuclear polarization at time t_n, $P_{He}(t_n)$	Decay time T_1

Background information on 3He-cell transmission correction

4. Calculation of correction parameters for the sample measurements:

Step Nr. 4 : is to define the polarization dependent transmission functions of each 3He cell (Polarizer, P, and analyzer, A):

$$T^{\pm}(t_n, \lambda) = \mathrm{TE} * \exp(-O(\lambda) \pm O(\lambda) * P_{He}(t))$$

$$\begin{pmatrix} I_{++} \\ I_{+-} \\ I_{-+} \\ I_{--} \end{pmatrix} = I_0 \cdot \begin{pmatrix} A_+ & A_- & 0 & 0 \\ A_- & A_+ & 0 & 0 \\ 0 & 0 & A_+ & A_- \\ 0 & 0 & A_- & A_+ \end{pmatrix} \cdot \begin{pmatrix} P_+ & 0 & P_- & 0 \\ 0 & P_+ & 0 & P_- \\ P_- & 0 & P_+ & 0 \\ 0 & P_- & 0 & P_+ \end{pmatrix} \cdot \begin{pmatrix} S_{++} \\ S_{+-} \\ S_{-+} \\ S_{--} \end{pmatrix}$$

To note:

(1) The transmission is only polarization dependent for an incoming polarized neutron beam, hence polarization dependence of the transmission needs to be taken into account only for the sample measurements, but not for determining the time-decay of each single 3He-cell

Fix input values	Transmission of empty glass, TE	Opacity, $O(\lambda)$	Time-stamp, t_n	Wavelength , λ
Neutron data input	Sample data of - full-polarized neutron beam, all four spin-channels - I^{++}, I^{+-} , I^{-+} , I^{--}			
Parameters to compute	Polarization-dependent transmissions through the cell - T+, T- (for polarizer and analyzer)	Corrected sample data - I^{++}_{corr} , I^{+-}_{corr} , I^{-+}_{corr} , I^{--}_{corr}		

Important information

1. Keep Wavelength-dependence for PA-correction
2. Normalization
   - normalization to monitor counts should be done before PA-correction
   - probably good to also normalize to all other background noise / detector efficiencies, etc. before PA-correction
   - think about: position of Monitors (for analyzer before, but for polarizer after cell?) → does that make a difference?
3. Difference of SM / 3He-cell usage:
   - Use same reduction script for any 3He-cell, independent of choice of polarizers
4. To think about:
   - 3D detector for SANS at DREAM – ask Celine/Wojtek/Mikhail how this would work
   - DB background same for using the 3He-cell or not? Is DB background polarization dependent?
   - Have to test this prior to operation, but consider it as same for now

Workflow for 3He + 3He – Option 2: 2 channels (W/o polarizer) + unpol

Measure parameters of both 3He cells
→ Opacity, pressure, initial polarization,…
→ To be fitted afterwards:

+

Sample: Measure 4-channels with sample
→ (w polarizer, w sample, w analyzer)
→ Do 15 min measurements (in our case)

+

3He:
(i) Measure unpolarized beam
→ Everything out, reference measurement
(ii) Measure I+ or I- (DB) (3He1)
→ (without polarizer)
(iii) Measure I+ or I- (DB) (3He2)
→ (without analyzer)
(iv) as 60s measurements
→ Good time-steps: 1h

E.g. following procedure

- 4-channel measurement on sample
  → Move sample in
  → Measure 15 mins x 4 channels (ca 1h loop)
- Unpol-measurement on DB (”unpol”)
- I+ or I- measurement on DB (”pol out”)
  → Move polarizer out
  → Measure 60 s x 2 channels
- I+ or I- measurement on DB (”an out”)
  → Move analzyer out
  → Move polarizer in
  → Measure 60 s x 2 channels

→**Loop** until good signal to noise ratio for the measurements

For future: workflows for Supermirror + 3He cell

Workflow for SM + 3He – Option 1: 4 channels – to be optimized

$$\begin{pmatrix} I^{++} \\ I^{+-} \\ I^{-+} \\ I^{--} \end{pmatrix} = I_0 \begin{pmatrix} A^{+} & A^{-} & 0 & 0 \\ A^{-} & A^{+} & 0 & 0 \\ 0 & 0 & A^{+} & A^{-} \\ 0 & 0 & A^{-} & A^{+} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1-F1 & 0 & F1 & 0 \\ 0 & 1-F1 & 0 & F1 \end{pmatrix} \begin{pmatrix} P^{+} & 0 & P^{-} & 0 \\ 0 & P^{+} & 0 & P^{-} \\ P^{-} & 0 & P^{+} & 0 \\ 0 & P^{-} & 0 & P^{+} \end{pmatrix} \begin{pmatrix} S^{++} \\ S^{+-} \\ S^{-+} \\ S^{--} \end{pmatrix}$$

P(t, λ) = Polarizer transmission

A(t, λ) = Analyzer transmission

F(λ) = Flipper efficiency

(1) Normalize data by counting time or the monitor counts.

(2) Functions:

$$A^{\pm}(t,\lambda) = \mathrm{TE} * \exp(-O(\lambda) \pm O(\lambda) * P_{He}(t))$$

$$P_{He}(t) = \mathrm{P_{He0}(t_0)} * \exp(-\frac{\Delta t}{\gamma})$$

A(t, λ) = Analyzer (3He) transmission

AP(t) = Atomic polarization

Known Values:

Opacity	$O(\lambda)$= 0.0733 $p\ l\ \lambda$
filling time	t_0
initial He-polarization	P_{He0} (t_0)
time-stamp	t_n

Unknown params to fit:

Base Intensity	I_0
Flipper efficiency:	$E_{F1}(\lambda)$
3He time-decay constant:	$T1$ [h]
Transmission unfilled cell:	TE

p	pressure of 3He cell
λ	neutron wavelength.
l	path length through the cell

Can be either pre-measured or fitted:

Polarizer transmission SM(+):	$P^{+}(\lambda)$
Polarizer transmission SM (-):	$P^{-}(\lambda) = 1-P^{+}(\lambda)$

Measure ***I*** → Fit $A^{\pm}(t,\lambda)$ → Insert into Matrix

Workflow for SM + 3He (MEOP) – Option 1: 4 channels

Measure parameters of 3He cell
→ Opacity, pressure, initial polarization,…
→ To be fitted afterwards:

+

Sample: Measure 4-channels with sample
→ (w polarizer, w sample, w analyzer)
→ Do 15 min measurements (in our case)

+

3He: Measure 4 channels without sample
→ (w polarizer, w analyzer)
→ Do 60s measurements
→ Max. time-steps: 2h (what we did at D33)
→ Good time-steps: 1h

E.g. following procedure (from D33 May 2023 Annika):

- 4-channel measurement on sample
  → Move sample in
  → Measure 15 mins x 4 channels (ca 1h loop)
- 4-channel measurement on DB
  →Move sample out
  →Measure 60 s x 4channels

→**Loop** until good signal to noise ratio for the measurements

Additionally to consider:

- Sample depolarization – effectively changes polarizer efficiency, but would still be nice to be able to insert if users know it?
  → Proposition: leave it out now, it would just come in as another matrix element with one additional factor
- At how many wavelength to measure?
  → Binning DB = sample binning

Workflow for SM + 3He – Option 2: 2 channels + unpol – to be optimized

Input Values:

filling time	t_0
time-stamp	t_n
Wavelength	λ
Polarizer transmission SM(+):	$P^{+}(\lambda)$
Polarizer transmission SM (-):	$P^{-}(\lambda) = 1\text{-}P^{+}(\lambda)$

Unknown params to fit:

Base Intensity	I_0
3He time-decay constant:	γ [h]
Transmission unfilled cell:	TE

(a) Either by measurement of pressure from ³He-team after filling:

$$O(\lambda) = 0.0733\, p\, l\, \lambda$$

(b) Or by neutron beam:

$$O(\lambda) = -ln[\frac{T^{unpol.beam}_{unpolarized\ ^3He\ cell} - T_{bg,\ He}}{T^{unpol.beam}_{^3He\ cell\ out} - T_{bg,\ noHe}}\frac{1}{TE)}]$$

2. Initial nuclear polarization

$$P_{He0}(t_0) = acosh[\frac{T^{unpol.beam}_{polarized\ 3He\ cell} - T_{bg,\ He}}{T^{unpol.beam}_{^3He\ cell\ out} - T_{bg,\ noHe}}\frac{1}{TE \cdot exp(O(\lambda))}]/O(\lambda)$$

3. Time-decay

$$P_{He}(t) = \mathrm{P_{He0}}(t_0) * \exp(-\frac{\Delta t}{T_1})$$

4. Determine correction factors for polarization dependent cell transmission

$$Transmission^{\pm}(t,\lambda) = \mathrm{TE} * \exp(-O(\lambda) \pm O(\lambda) * P_{He}(t))$$

Workflow for SM + 3He – Option 2: 2 channels (W/o polarizer) + unpol

Measure parameters of 3He cell
→ Opacity, pressure, initial polarization,…
→ To be fitted afterwards:

+

Sample: Measure 4-channels with sample
→ (w polarizer, w sample, w analyzer)
→ Do 15 min measurements (in our case)

+

3He:
(i) Measure unpolarized beam
→ W/o polarizer, w/o analyzer, w/o sample
(ii) Measure I^+ or I^-
→ (without polarizer, with analyzer)
(iii) Loop as 60s measurements
→ Good time-steps: 1h

E.g. following procedure

- 4-channel measurement on sample
  → Move sample in
  → Measure 15 mins x 4 channels (ca 1h loop)
- Unpol measurement on DB (Tunpol, 3He out)
  →Move polarizer out
  →Move analyzer out
  →Measure 60 s
- I^+ or I^- measurement on DB (3He in)
  →Move analzyer in
  →Measure 60 s x 2 channels

→**Loop** until good signal to noise ratio for the measurements