Introduction to PNR

NIST Center for Neutron Research

CHRNS
CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING

What is PNR For?

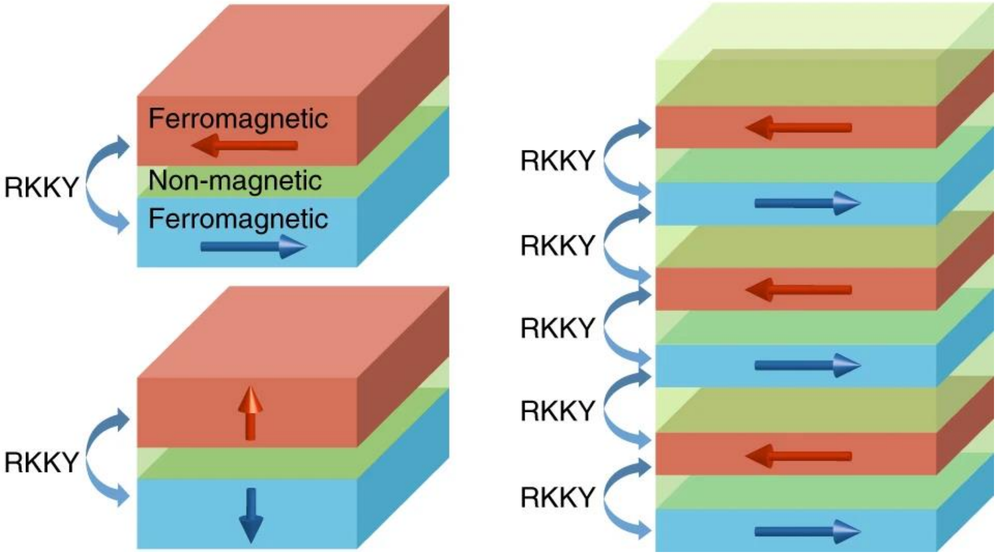
Magnetometry

Measures entire sample, reports aggregate properties

Electrical Transport

Probes conductive layers preferentially. Interpretation complex, not quantitative

What if we have a multilayer structure? A GMR stack, for example?



R. A. Duine et al., Nature Physics ***14****, 217 (2018)*

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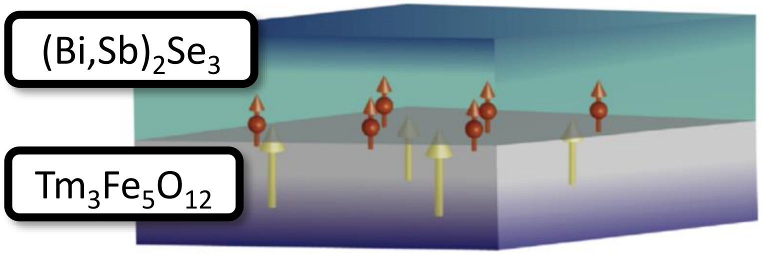

C. Tang et al., Science Advances 3, e1700307 (2017)

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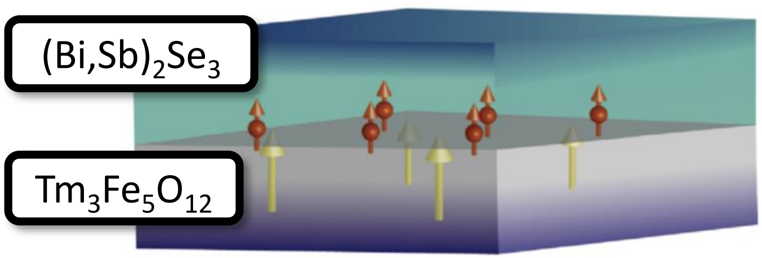

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Magnetic X-ray Spectroscopy

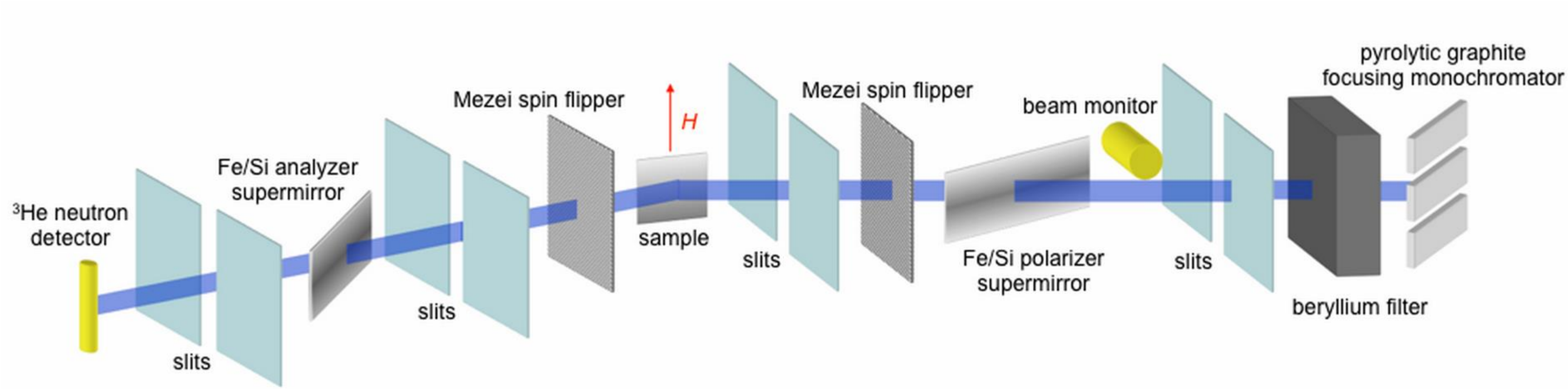
Element-specific magnetic characterization

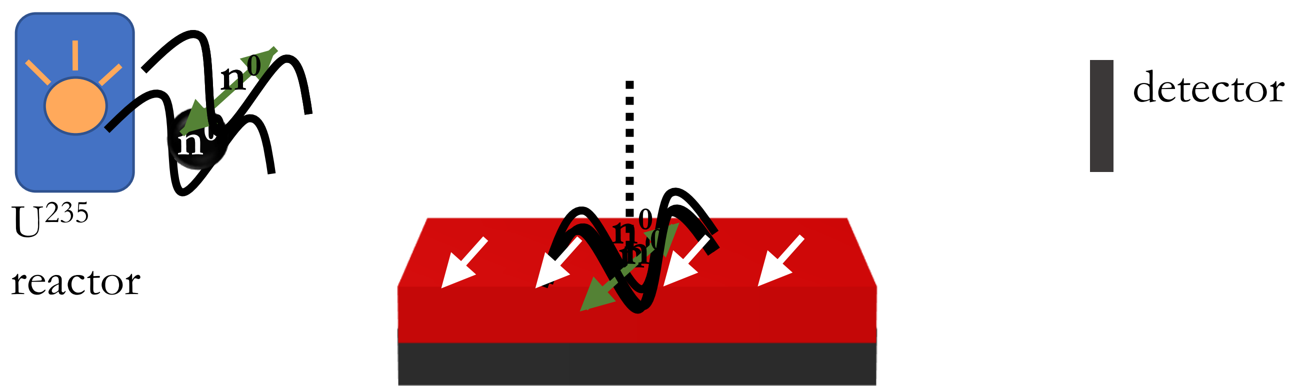
Polarized Neutron Reflectometry

Depth-resolved magnetic characterization

- Which layers are magnetic?
- What direction are they pointing?
- Dead layers? Proximity Effects? Interface exchange coupling?

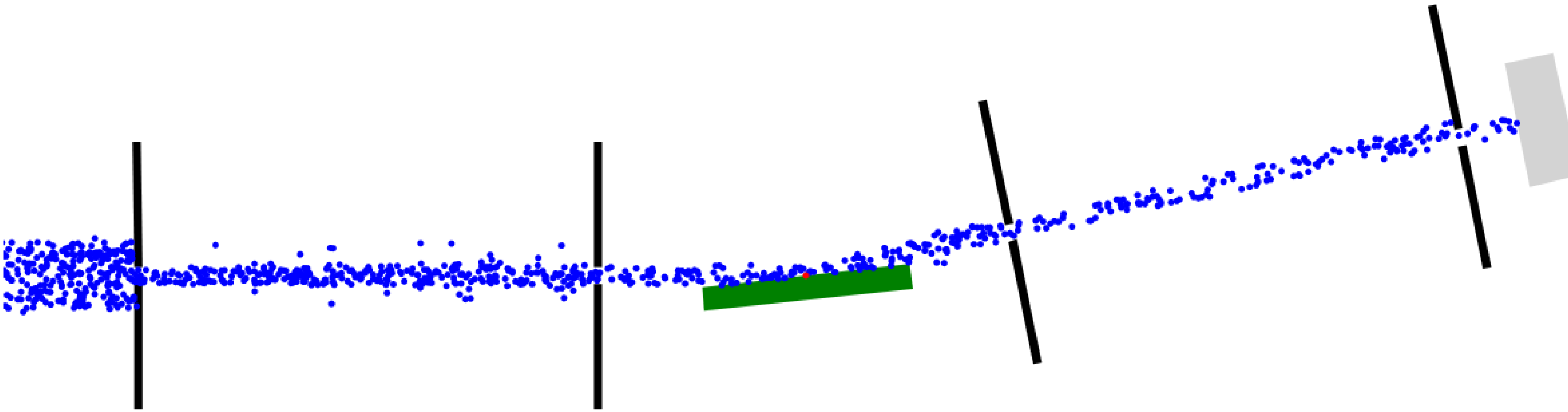
PNR Setup and Geometry





Web Tool: Pretend Reflectivity

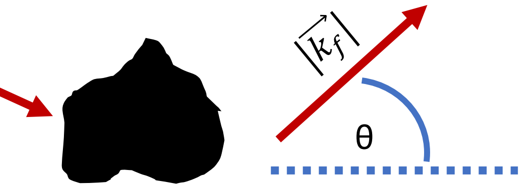
https://ncnr.nist.gov/instruments/magik/d3-science/reflectometer_alignment_sim.html



Because is a scattering technique where collect data as a function of angle, this is a **reciprocal space** technique

Written and supported by Dr. Brian Maranville

Neutron Reflectometry Data



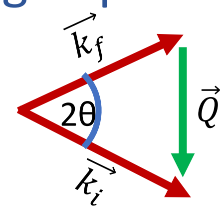
Incident wave vector with

$$|\overrightarrow{k_i}| = \frac{2\pi}{\lambda_i}$$

$\vec{Q} = \overrightarrow{k_i} - \overrightarrow{k_f}$ is the scattering vector

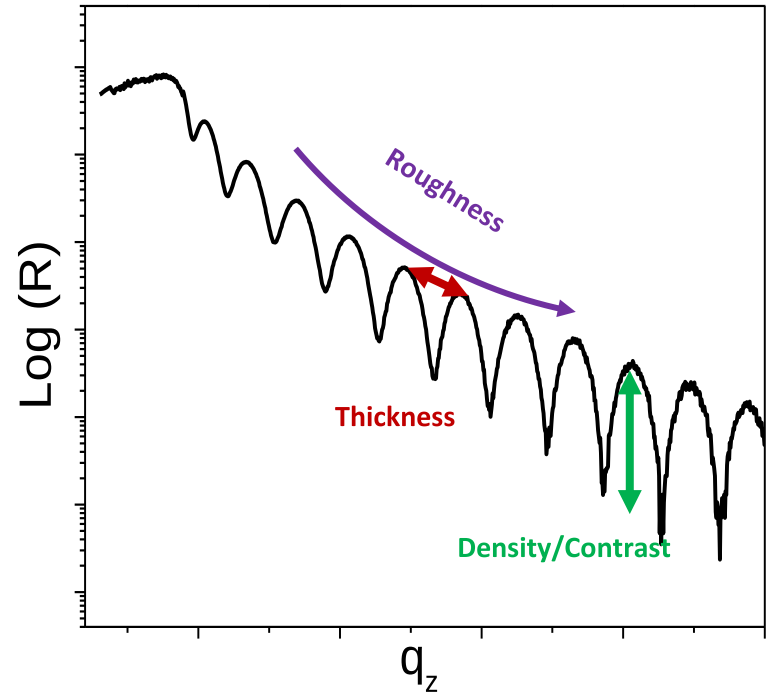
Elastic scattering implies:

$$k_i = k_f$$



$$Q = \frac{4\pi}{\lambda} \sin\theta$$

$$d \approx \frac{2\pi}{Q}$$



Neutron reflectometry is sensitive to chemical and in-plane magnetization depth dependence

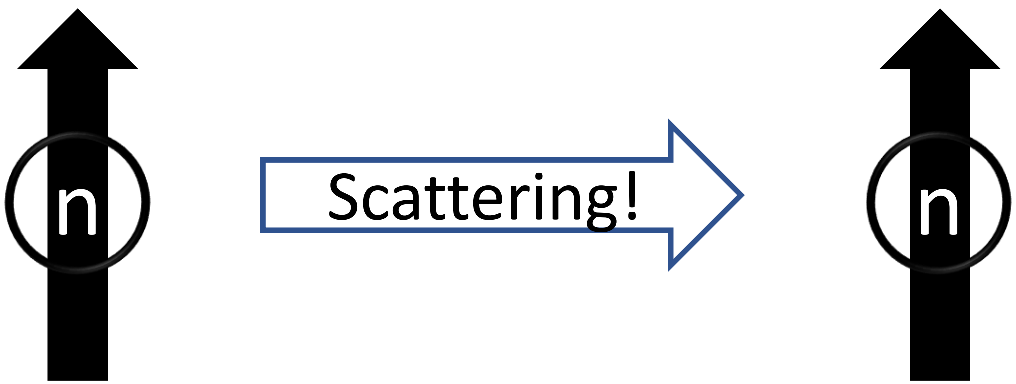
Polarization and Magnetism

Interacts with *Magnetic Fields*

Spin ½

$$\vec{\mu}_{\rm n} = -1.913\ \mu_{\rm N}\vec{\sigma}$$

Polarization Analysis:



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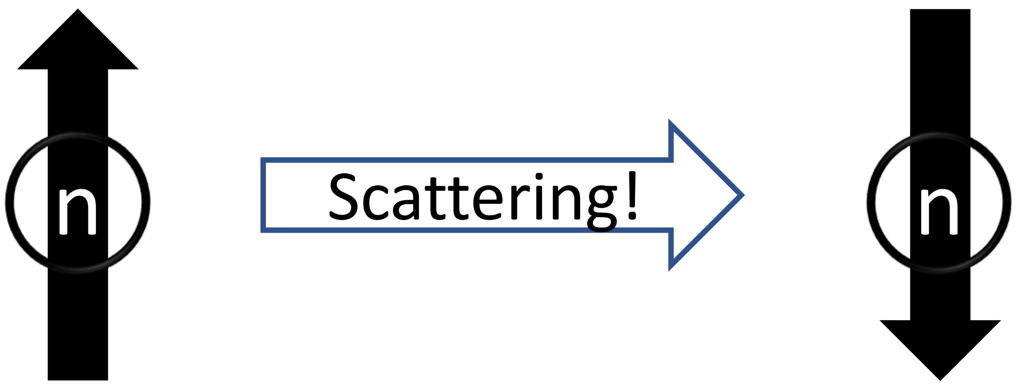

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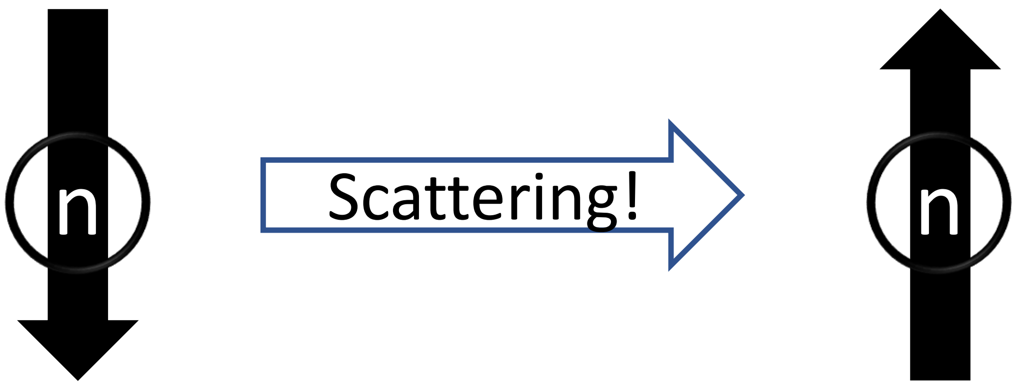

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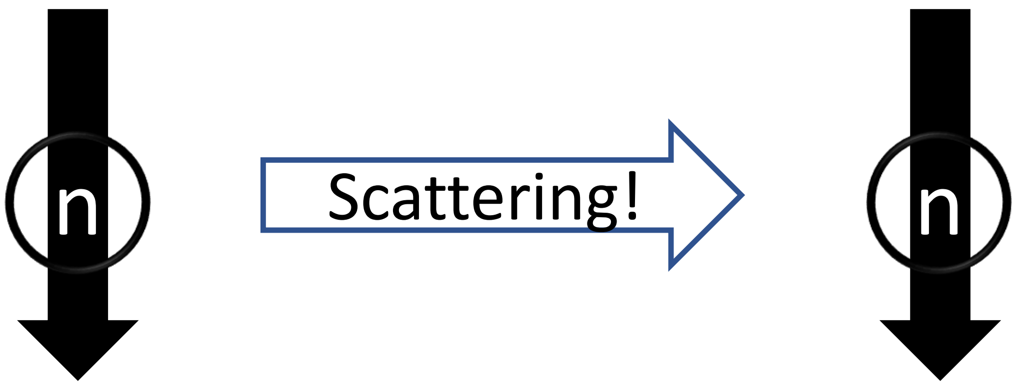


Polarization and Magnetism

Magnetic Sensitivity:

Non-spin flip (↑↑ or ↓↓)

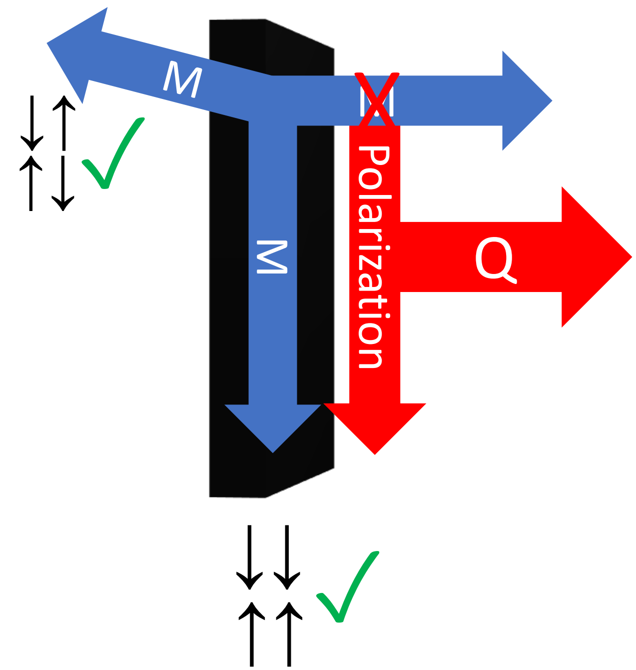
- M ∥ H

Spin-flip (or ↓↑)

- M ⊥ H

Both Cases

- M ⊥ Q



Continuum Limit:

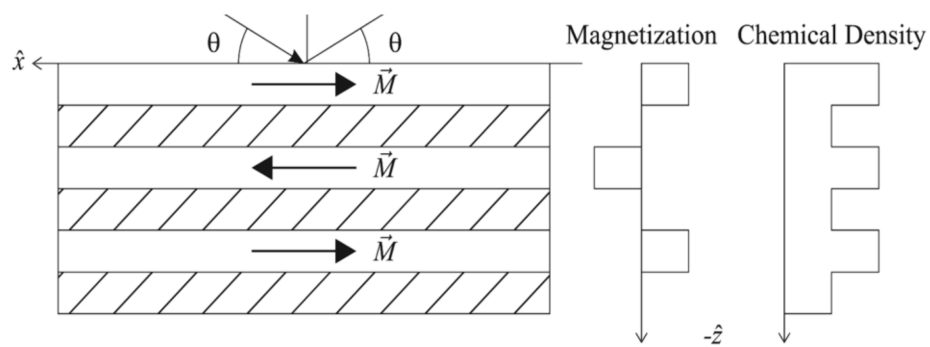
Scattering Length Density (SLD)

$\mathrm{SLD}_{\uparrow\uparrow} = \rho_N(Z) + \rho_M(Z)$

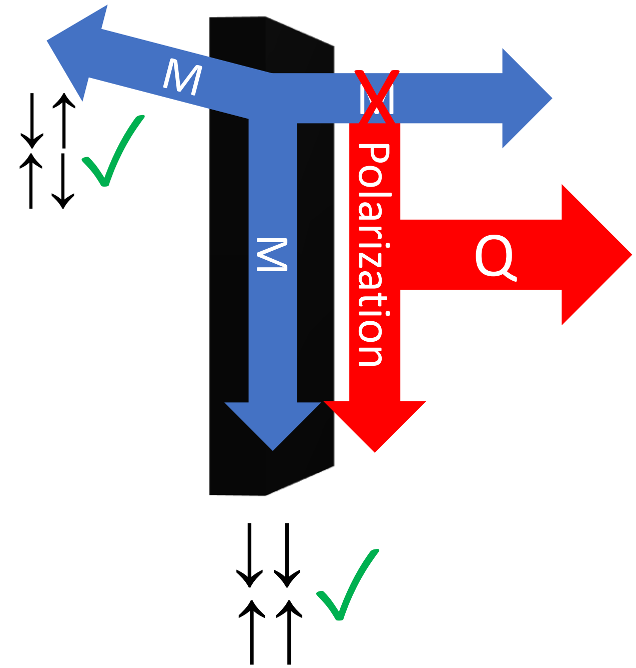
$\mathrm{SLD}_{\downarrow\downarrow} = \rho_N(Z) - \rho_M(Z)$

$$\rho_N = \sum_{j=1}^{M} N_j b_j$$

$$\rho_M = \mp \frac{m}{2\pi\hbar^2} \mu B$$



Polarization and Magnetism



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$$\rho_N = \sum_{j=1}^{M} N_j b_j$$

$$\rho_M = \mp \frac{m}{2\pi\hbar^2}\mu B \rightarrow \mathbf{M} = \rho_M/(2.853\times10^{-9}\ \text{Å}^{-2}\ \text{cm}^3/\text{emu})$$

Common SLD Values

Fitzsimmons and Majkrzak: https://www.ncnr.nist.gov/instruments/pbr/references/Fitz.pdf

Table 1 Listing of common elements and their neutron nuclear and magnetic scattering length densities.

Material	Number density, N [$Å^{-3}$]	Nuclear scattering length, b [Å]	Magnetic moment, μ [μ_B]	Nuclear scattering length density, ρ_n [$Å^{-2}$]	Magnetic scattering length density, ρ_m [$Å^{-2}$]
Ag	5.86 x10^{-2}	5.92 x10^{-5}		3.47 x10^{-6}	
Al	6.02	3.45		2.08	
Al_2O_3	2.13	24.4		5.21	
Au	5.90	7.90		4.66	
Co	9.09	2.49	1.715	2.26	4.12 x10^{-6}
Fe	8.47	9.45	2.219	8.00	4.97 x10^{-6}
FeF_2	2.75	20.76		5.71	
Fe_2O_3 (hematite)	2.00	36.32		7.26	
Fe_3O_4 (magnetite)	1.35	51.57	4.1	6.97	1.46 x10^{-6}
GaAs	2.21	13.87		3.07	
$LaAlO_3$	1.84	29.11		5.34	
$LaFeO_3$	1.65	35.11		5.78	
$LaMnO_3$	1.71	21.93		3.75	
MgF_2	3.07	16.68		5.12	
MgO	5.35	11.18		5.98	
MnF_2	2.58	7.58		1.96	
Nb	5.44	7.05		3.84	
Ni	9.13	10.3	0.604	9.40	1.46 x10^{-6}
^{58}Ni	9.13	14.4	0.604	13.14	1.46 x10^{-6}
^{62}Ni	9.13	-8.7	0.604	-7.94	1.46 x10^{-6}
$Ni_{81}Fe_{19}$	8.93	10.14	1.04	9.06	2.46 x10^{-6}
NiO	5.49	16.11		8.84	

Continuum Limit:

Scattering Length Density (SLD)

$SLD_{\uparrow\uparrow} = N(Z) + M(Z)$

$SLD_{\downarrow\downarrow} = N(Z) – M(Z)$

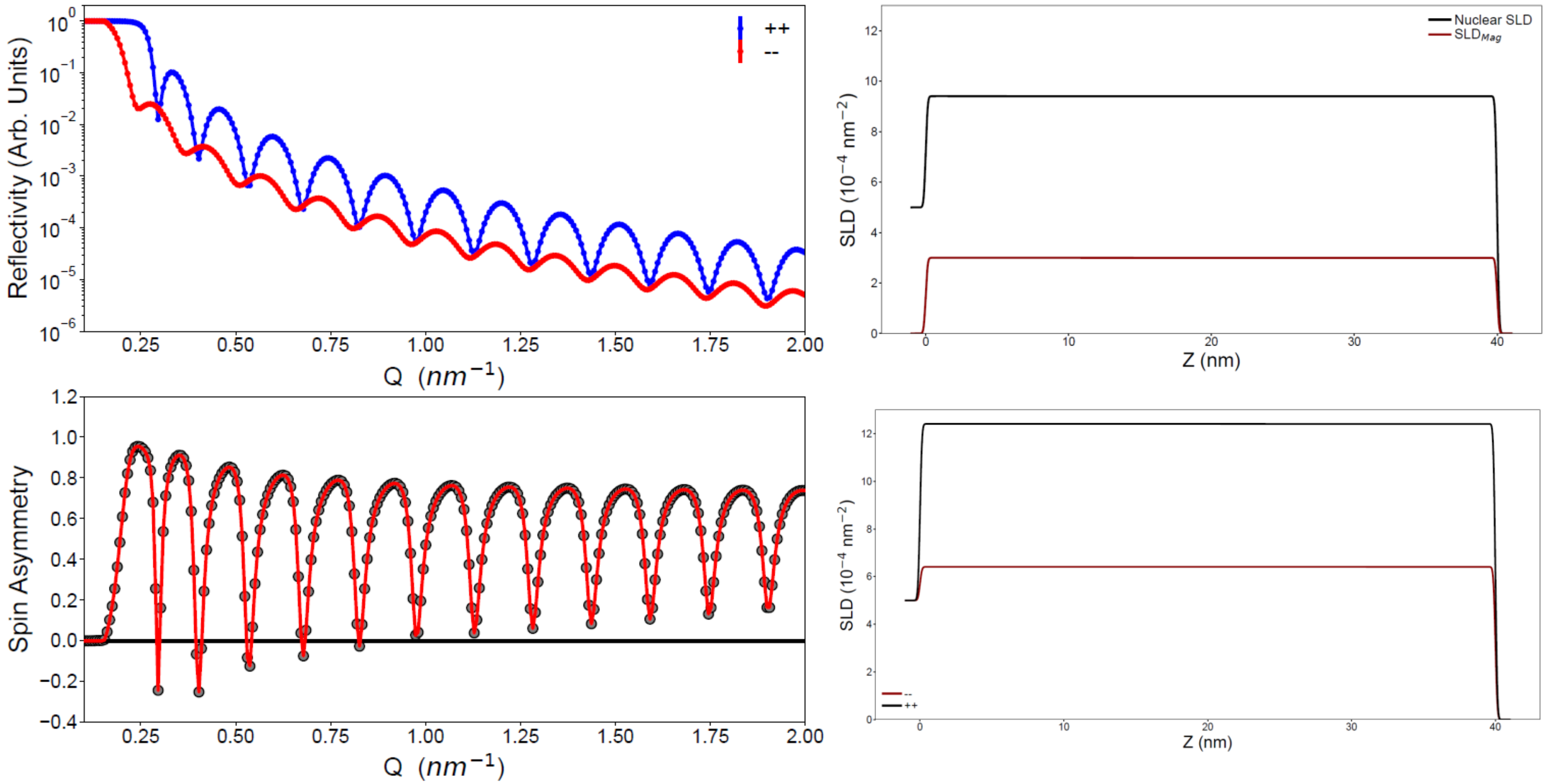
$R = (N + M)^2 = N^2 + 2NM + M^2$

$SA = (\uparrow\uparrow - \downarrow\downarrow)/(\uparrow\uparrow + \downarrow\downarrow) = 2NM/(N+M)^2$

Where N and M are the Fourier transform of the ρ_N and ρ_M profiles.

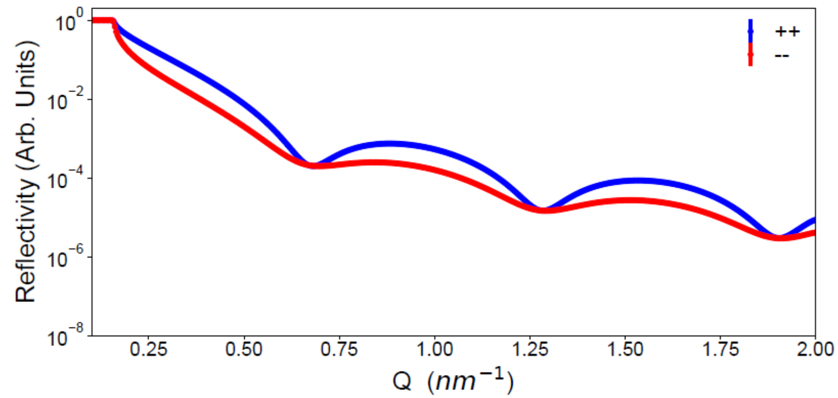
More complicated at the "Critical Edge"

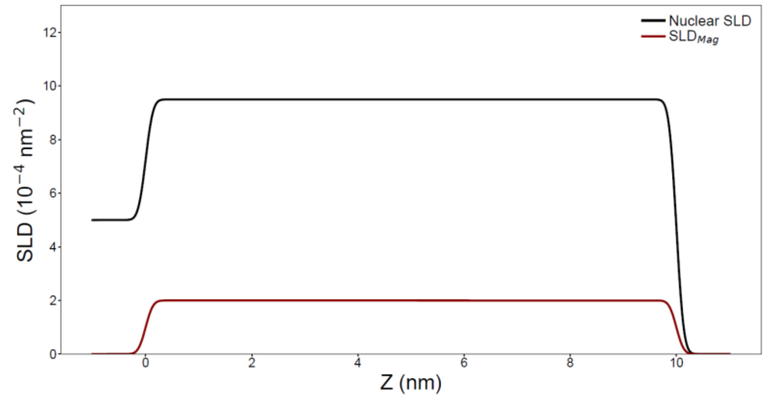
What should data look like?

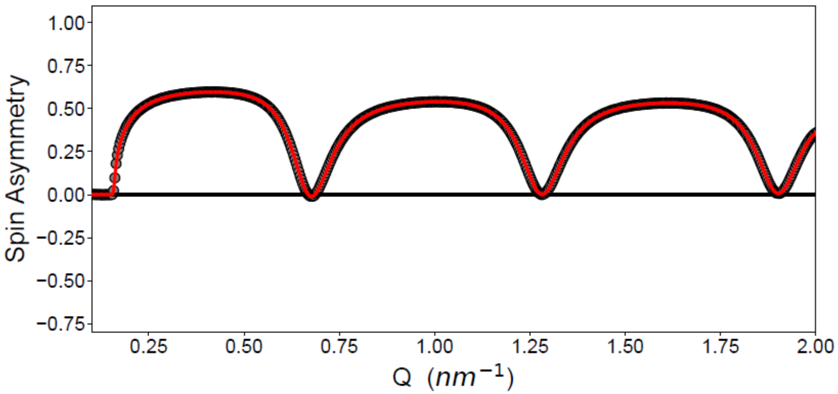


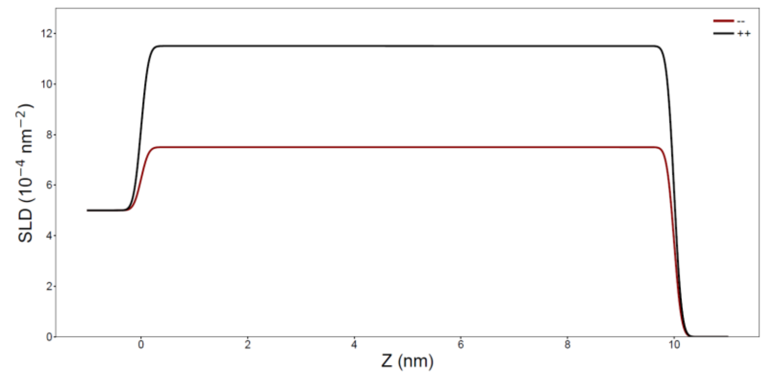
Here we see the simulated reflectivity of a 40 nm thick Ni film on MgO over a Q-range of 2 nm^{-1}

What should data look like?









Same system, but 10 nm instead of 40 nm

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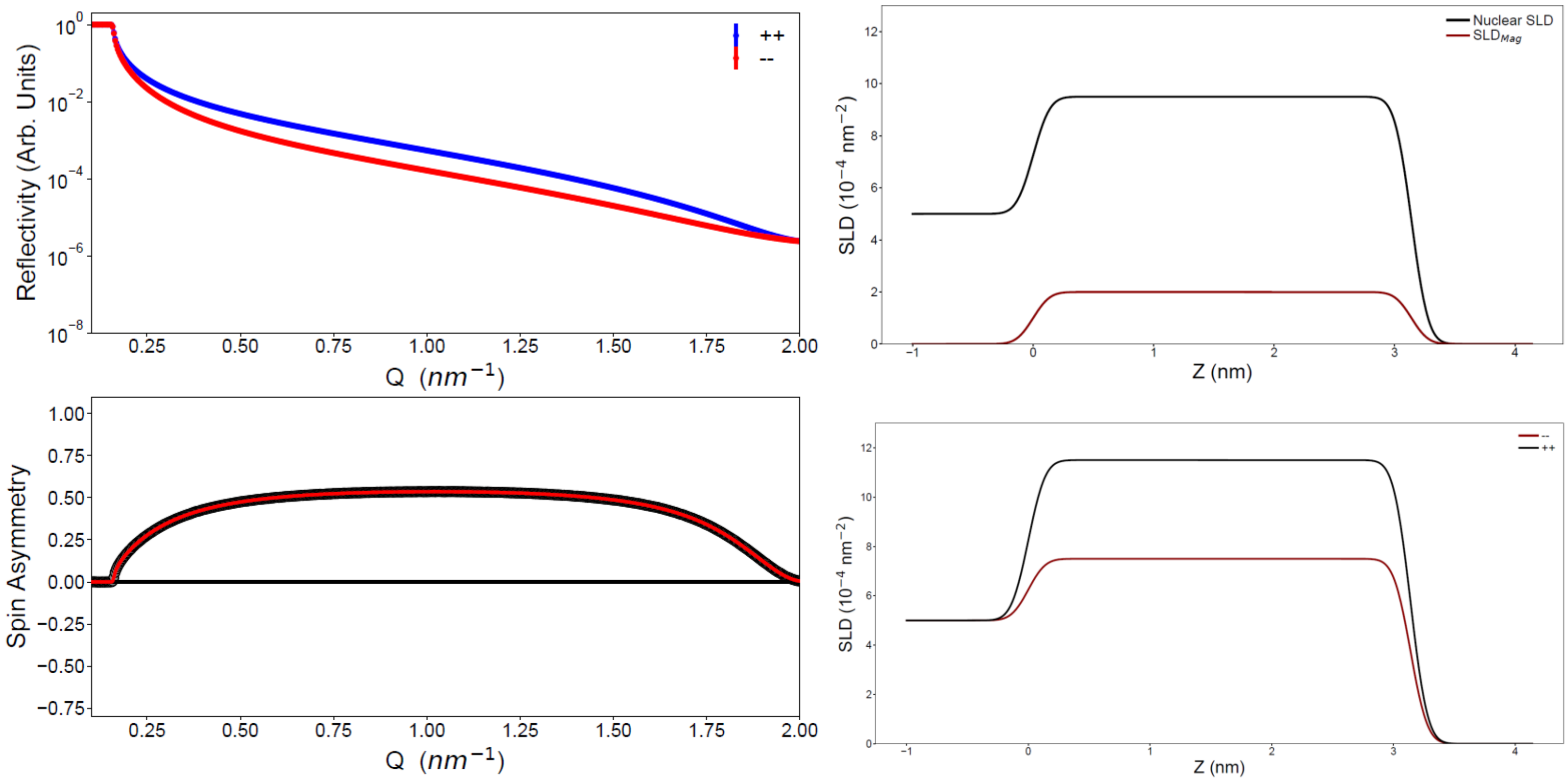
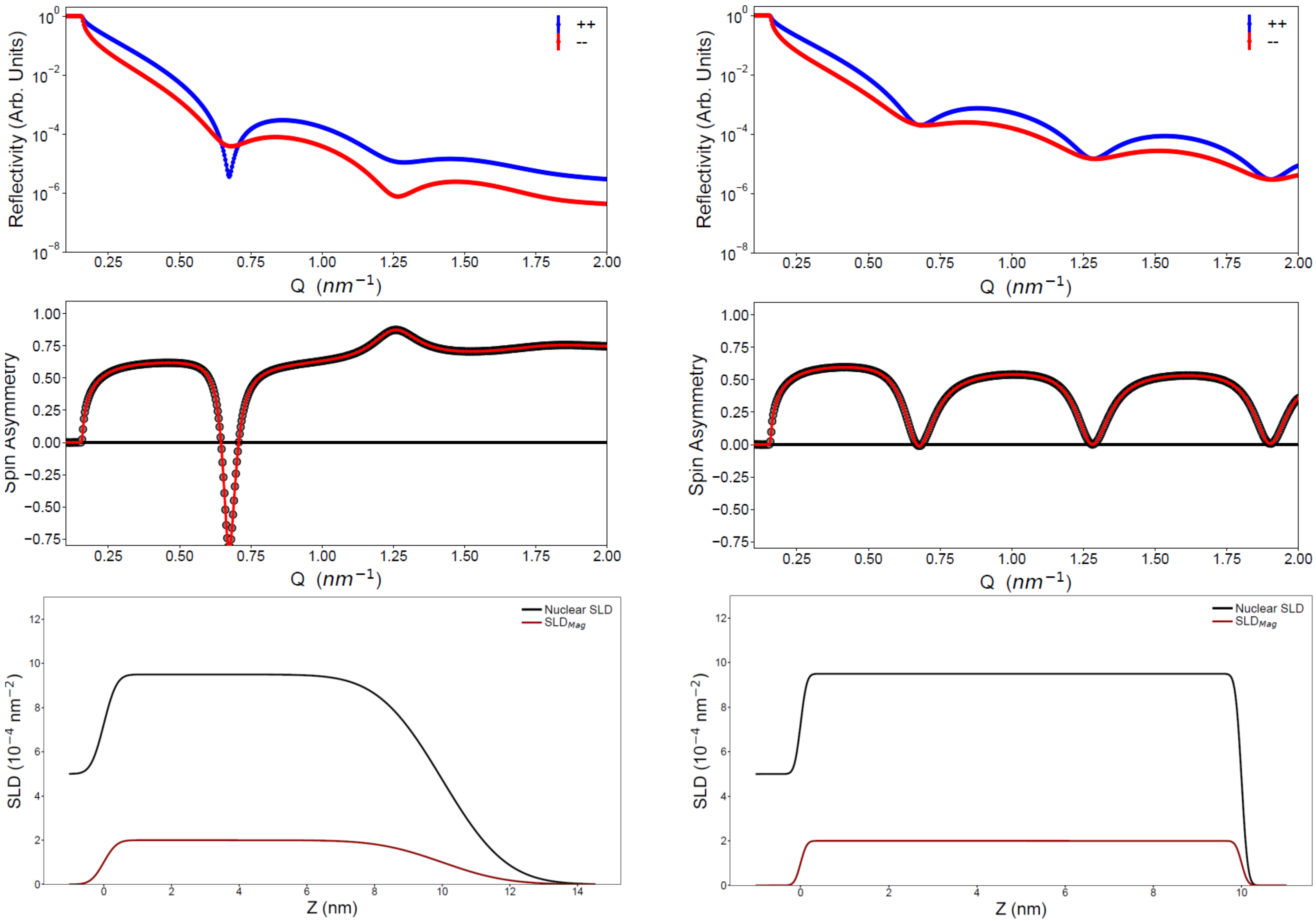
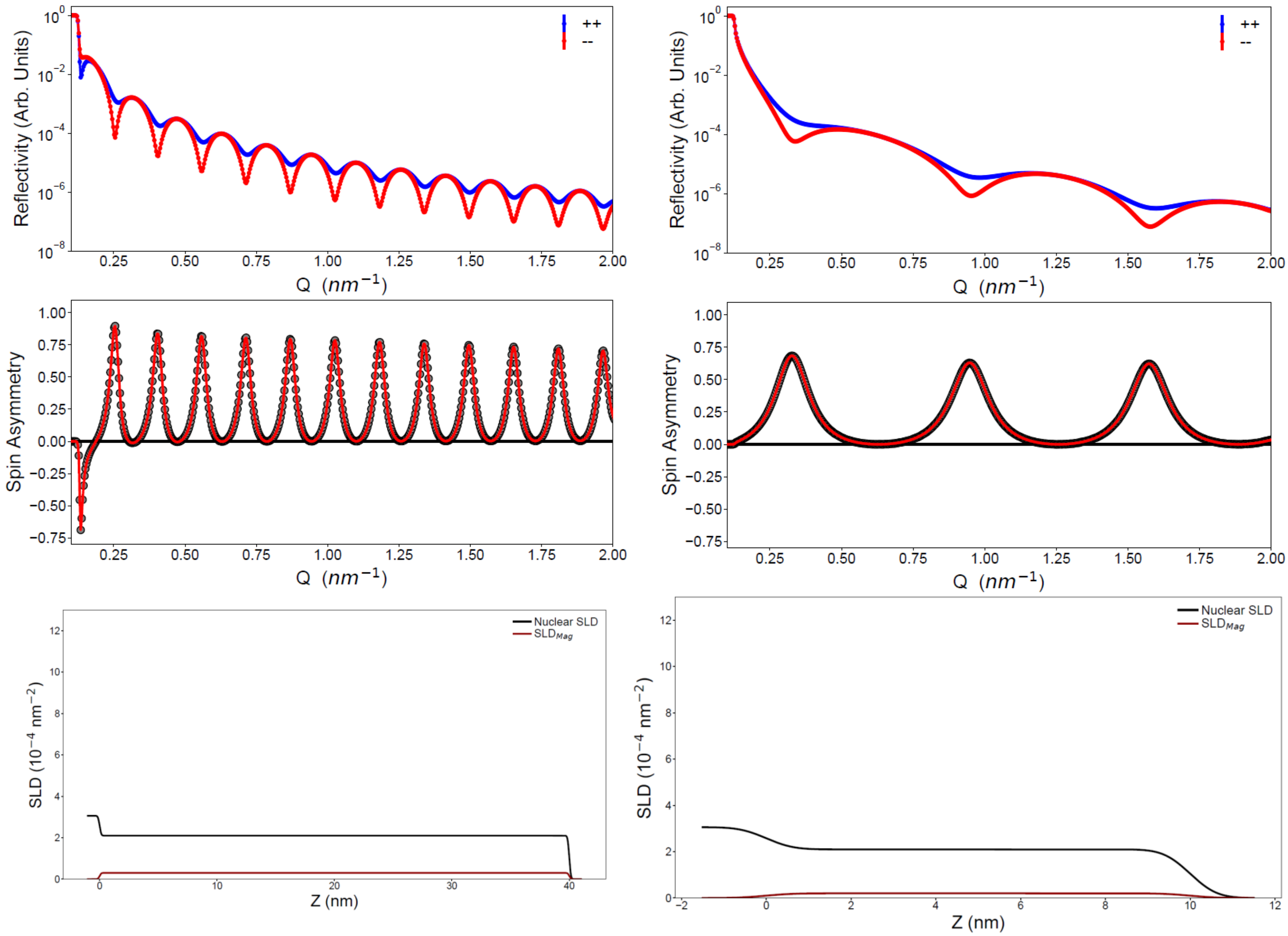


Same system, but 3 nm instead of 10 nm

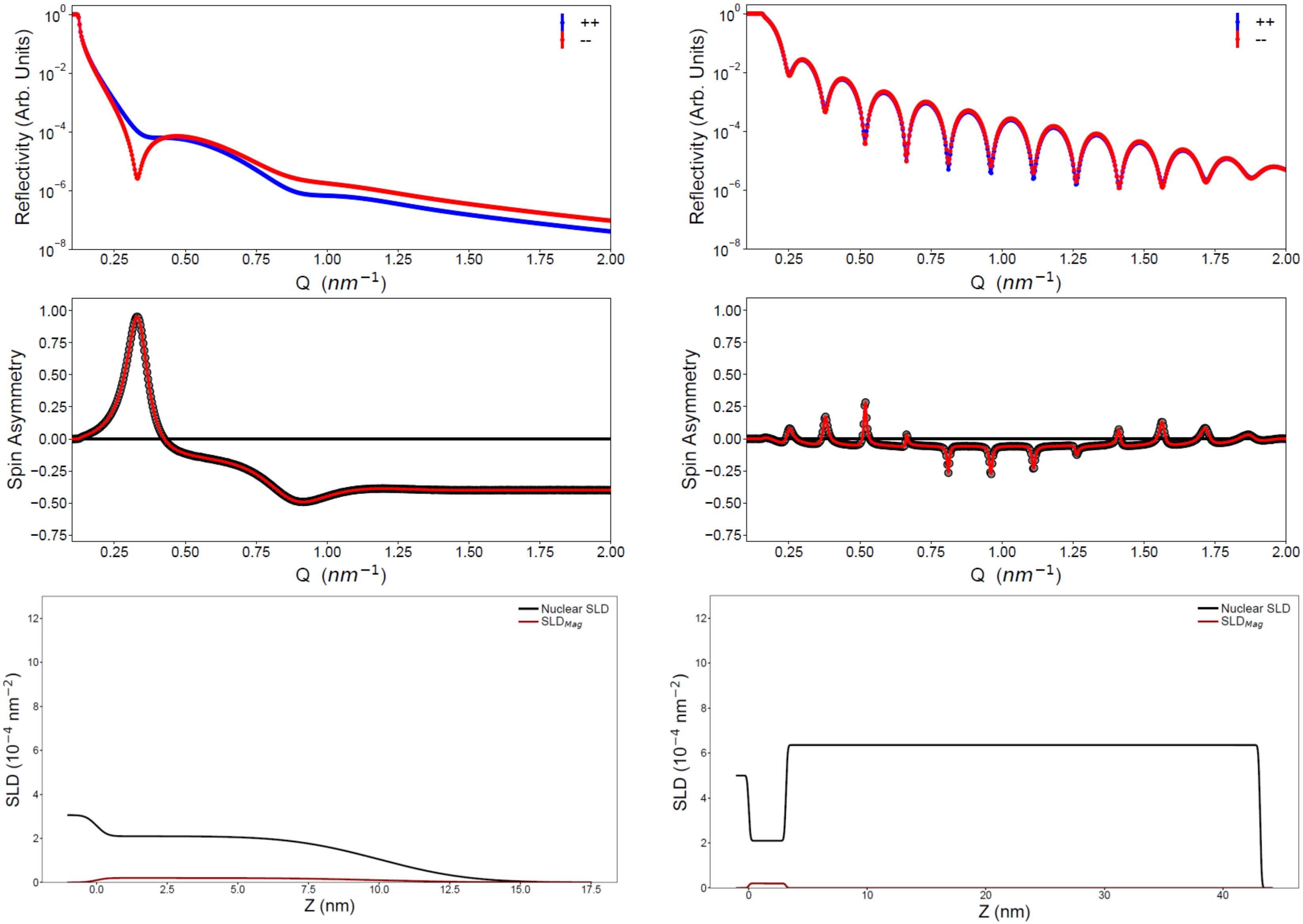
Roughness Dependence



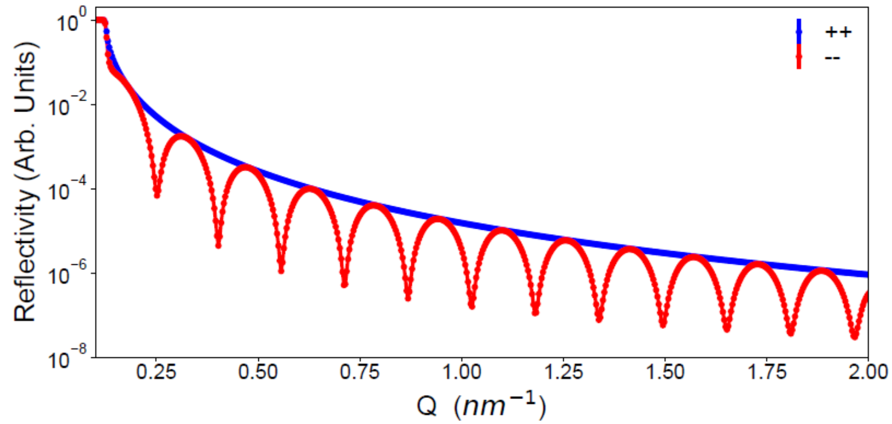
$Cr:(Bi,Sb)_2Te_3/GaAs$

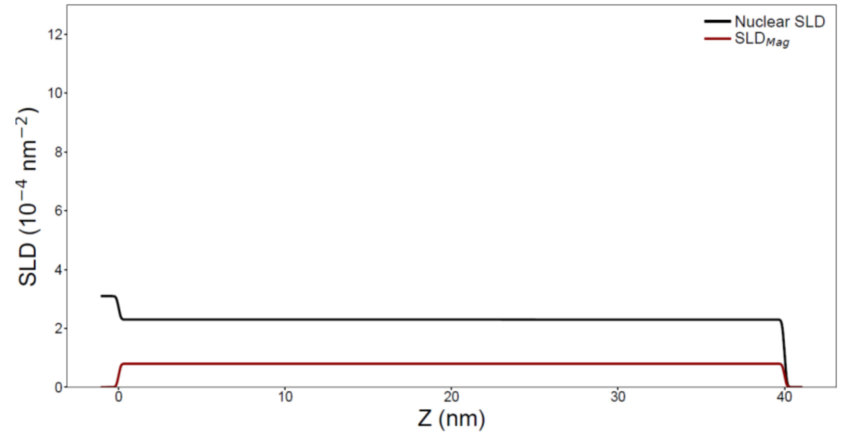


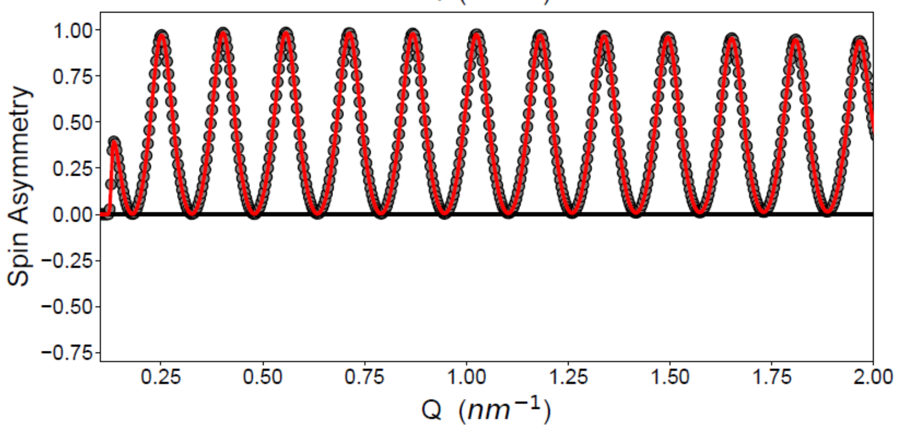
Difficult (Real) Cases

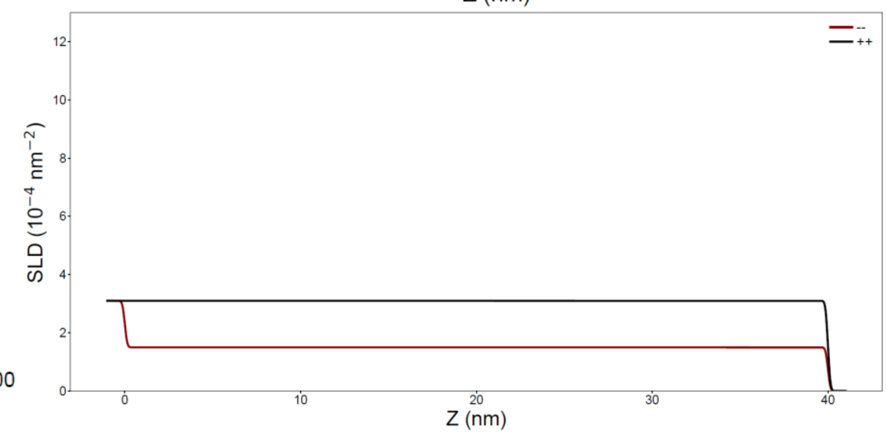


More Complex Examples



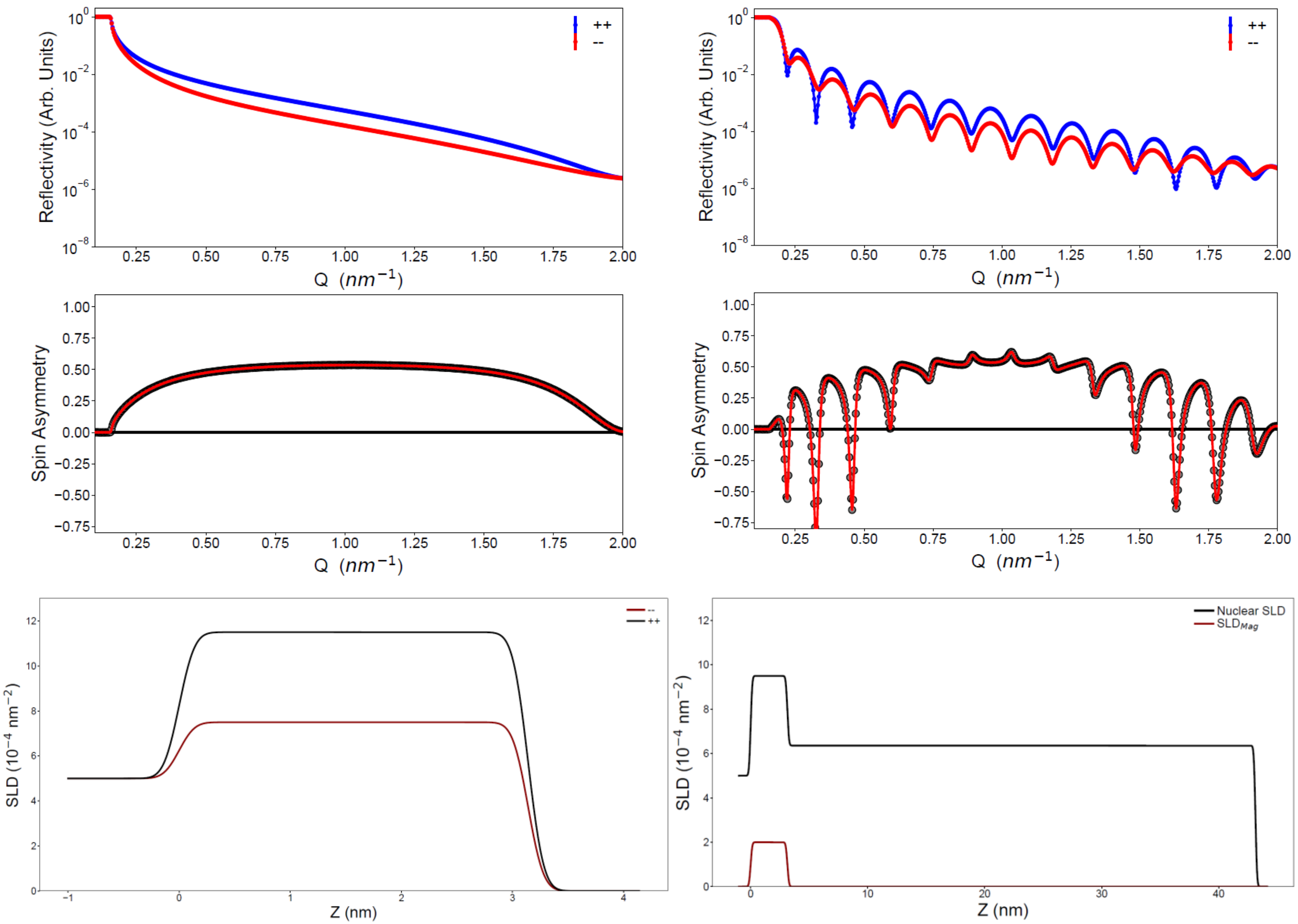






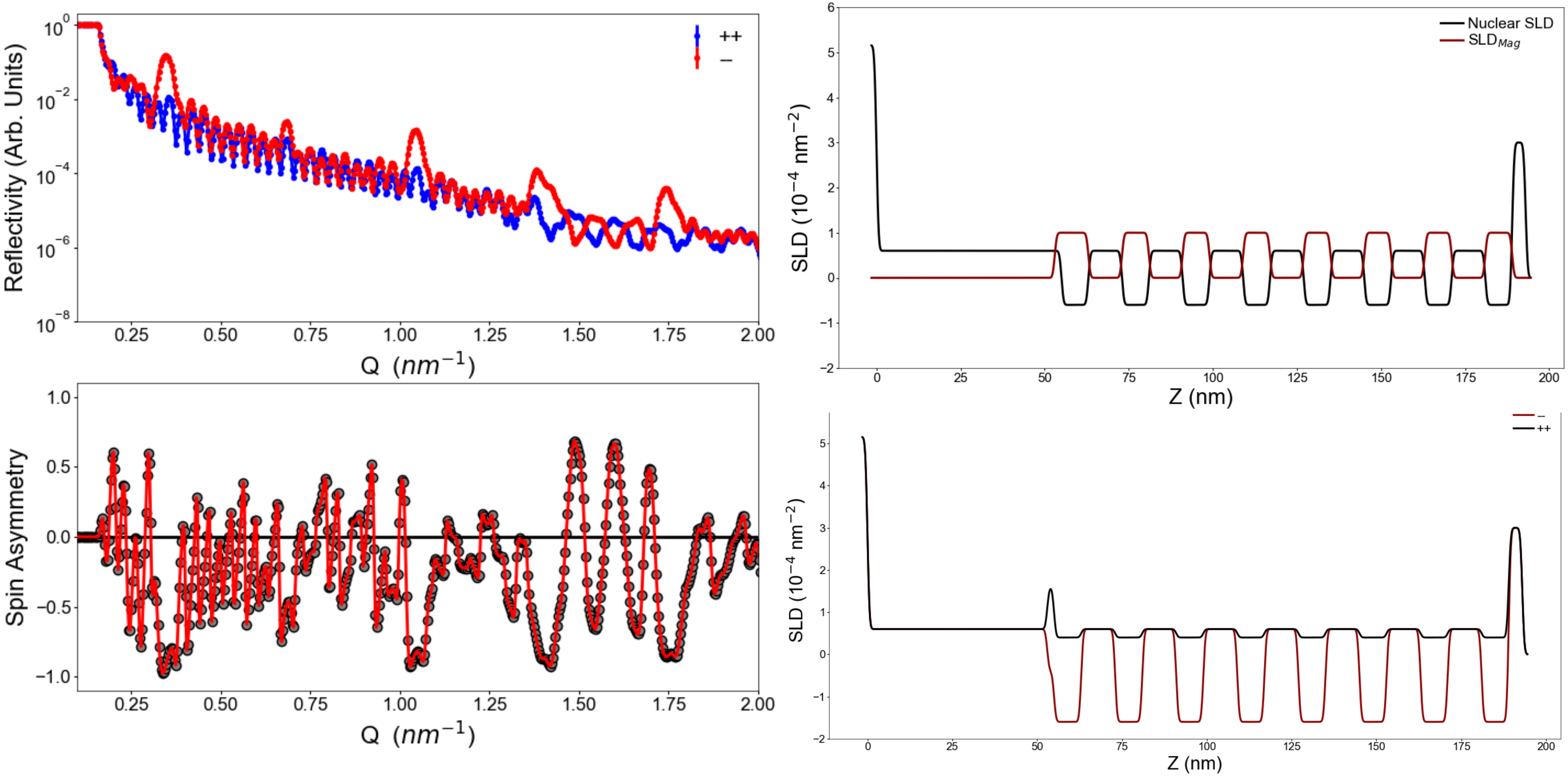
One can sometimes find systems where $\rho_N^{Substrate} = \rho_N^{Film} + \rho_M^{Film}$ for one of the two spin states. In this case we expect oscillations in one of the spin-states and a $R \sim Q^{-4}$ dependence for the other.

More Complex Examples



Here we see that the thick capping layer creates high-frequency features in the spin asymmetry, but the envelope function associated with the magnetic layer remains.

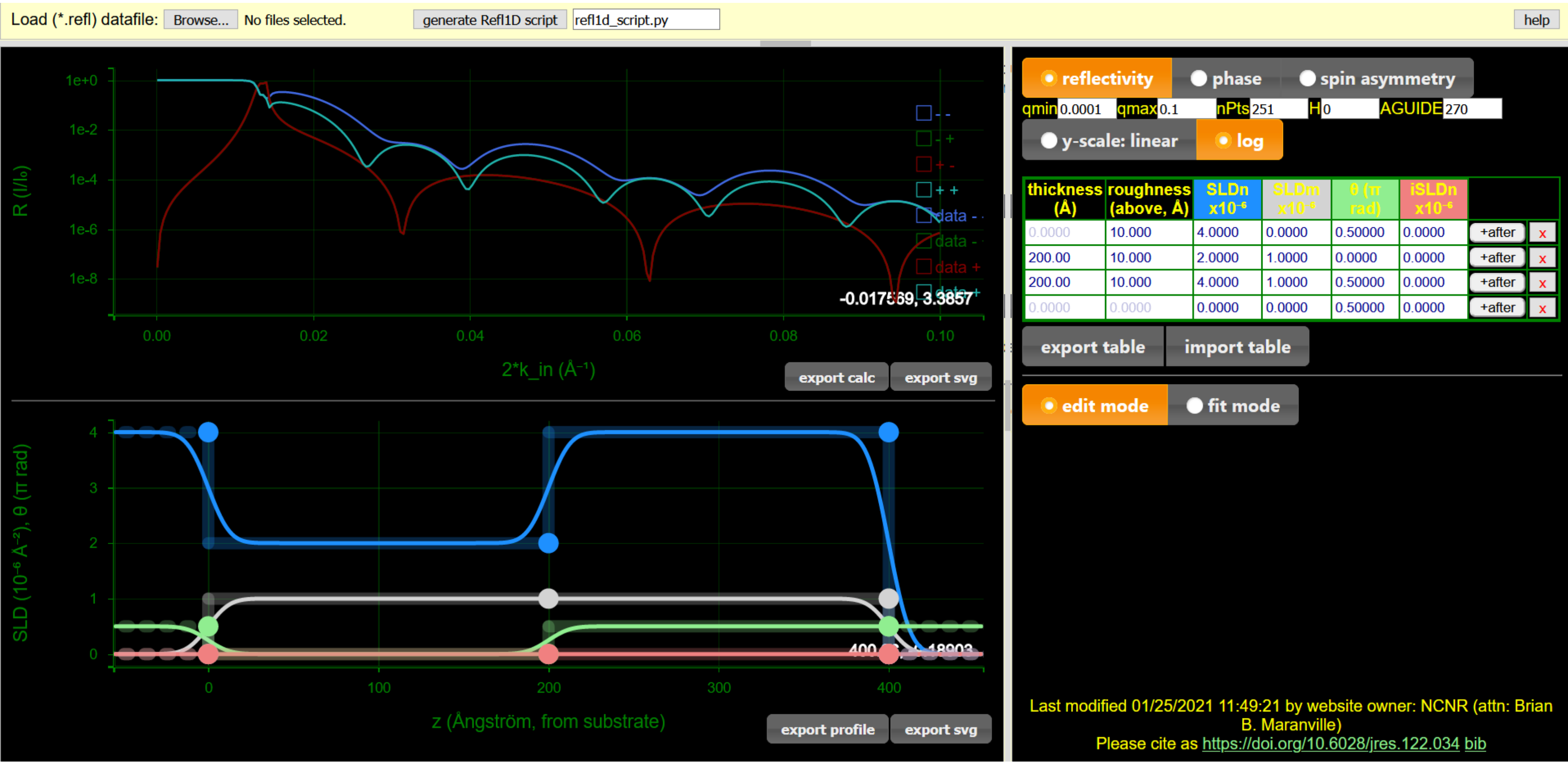
Superlattice



- Information-rich superlattice peaks (Bragg reflections)
- Negative scattering length density is a real thing

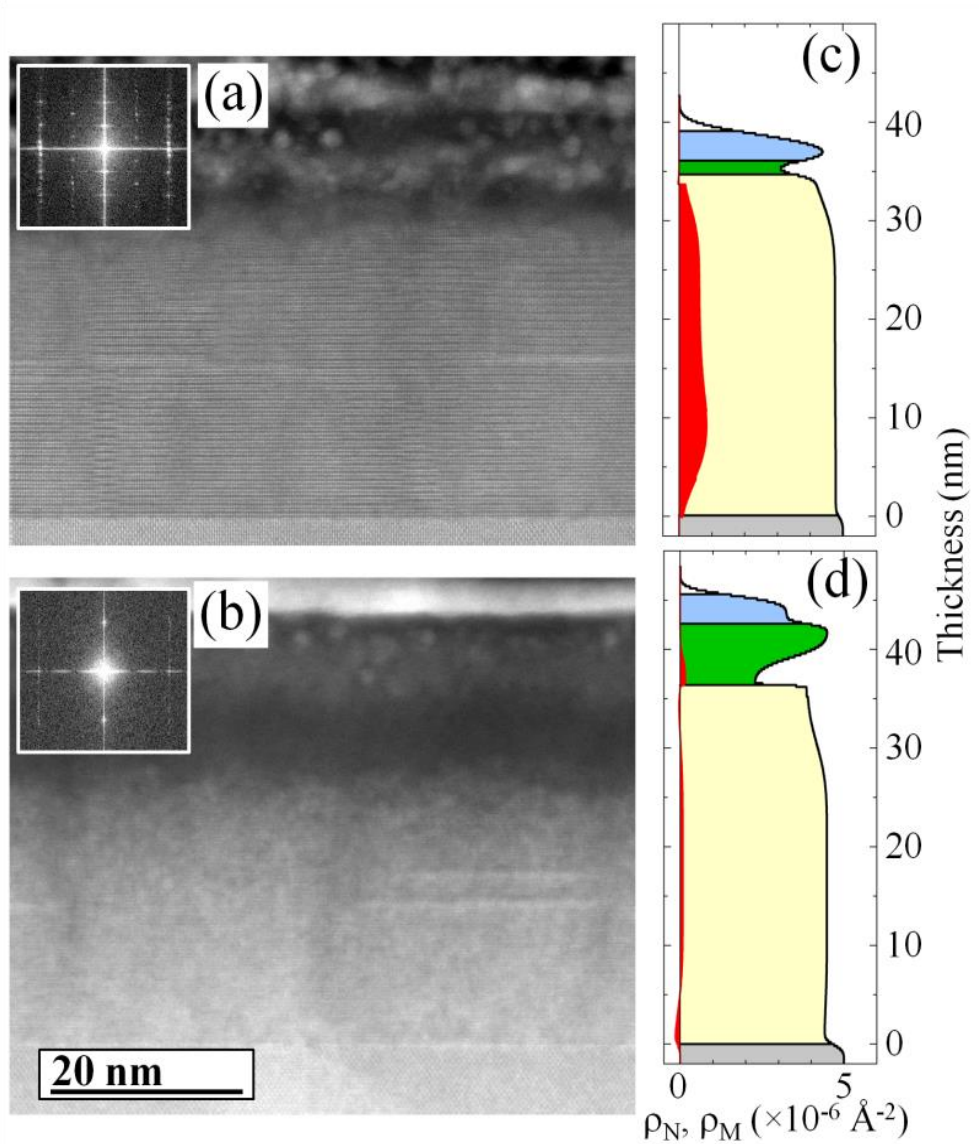
Simulation Tool

https://www.ncnr.nist.gov/instruments/magik/calculators/calcR_mag_d3_dark.html



Written and supported by Dr. Brian Maranville

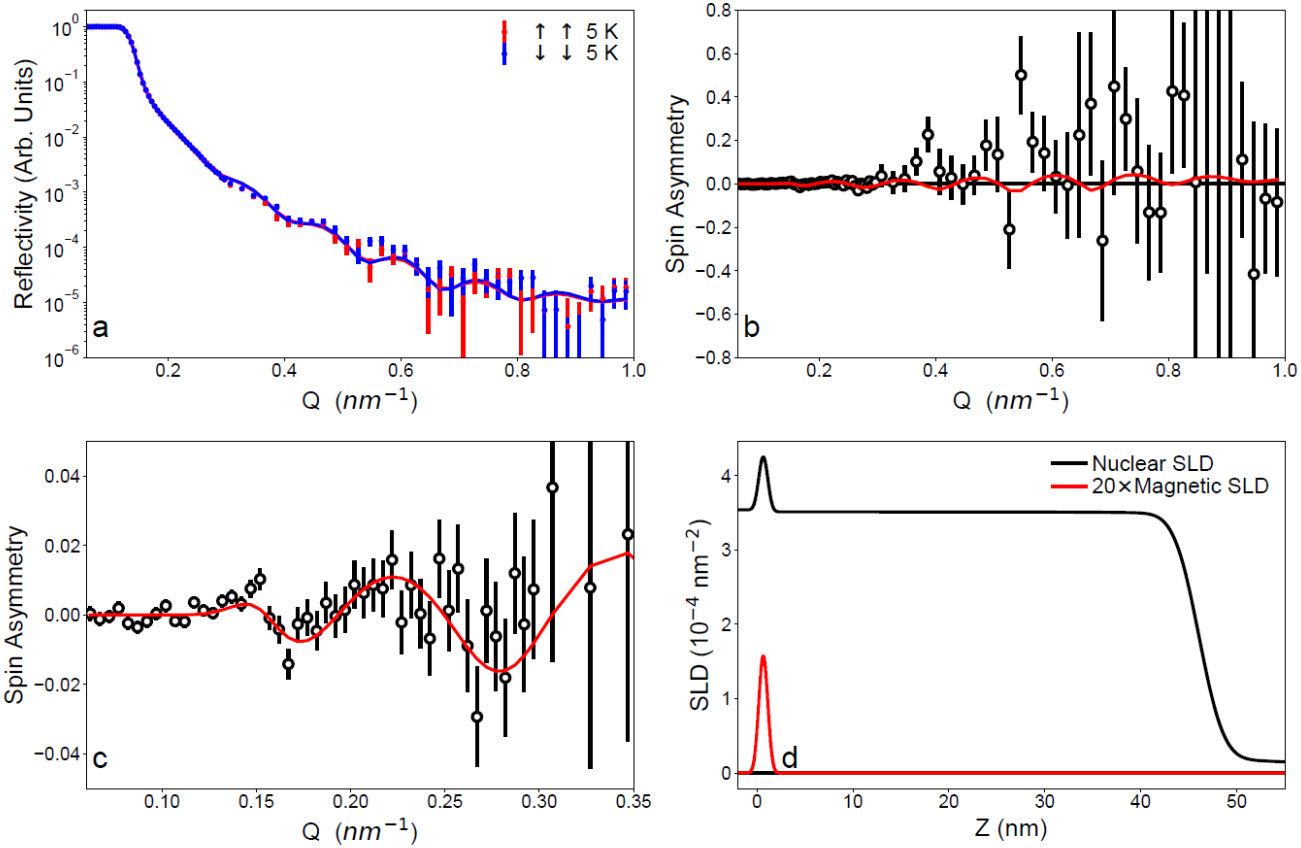
Should We Trust PNR?



- PNR provides extremely accurate depth profiles
  - Structural
  - Magnetic
- Can ALSO extract parameters like density/composition
- Sensitive enough to detect ~3% variations in oxygen content

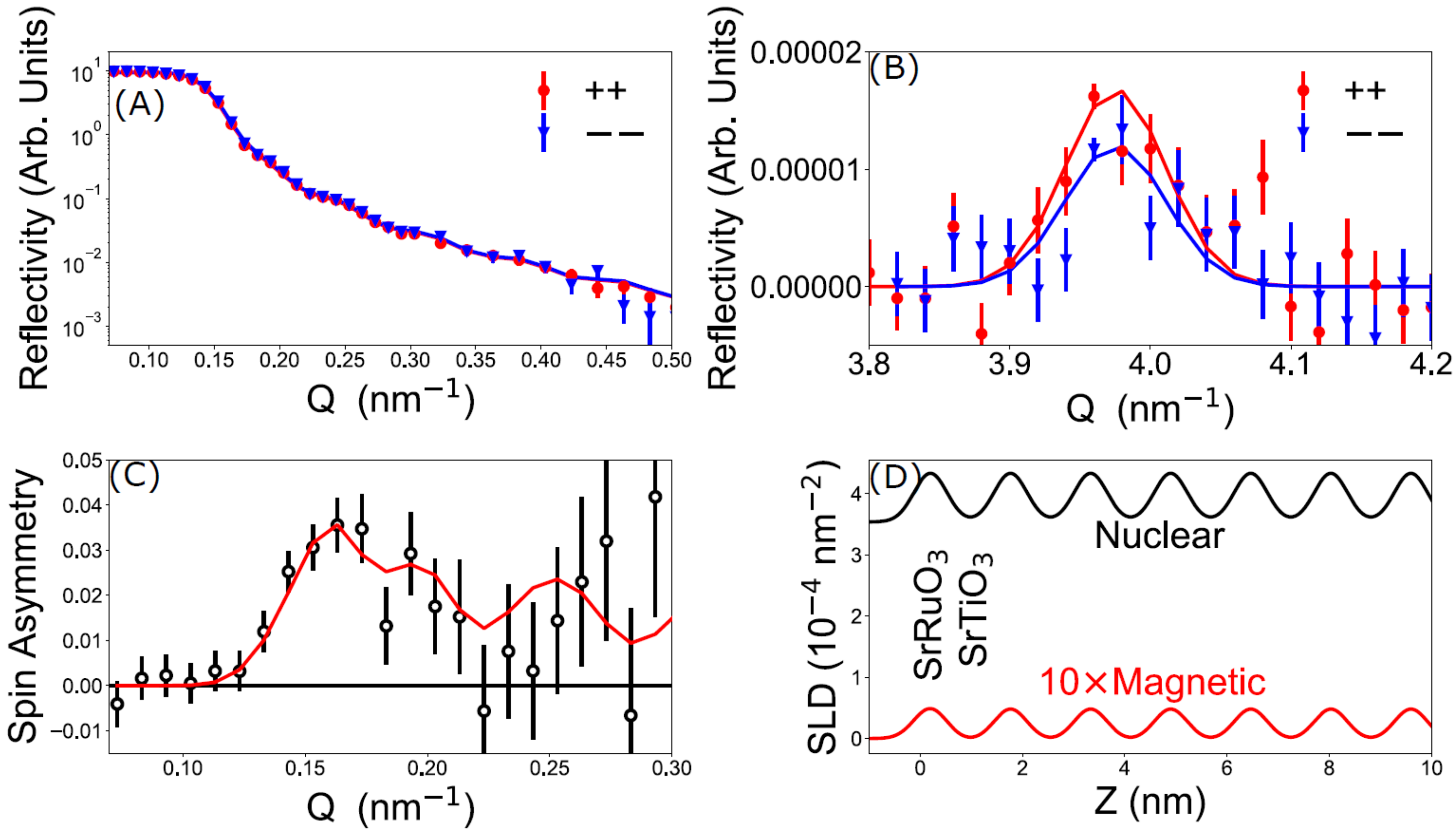
D. A. Gilbert et al., *Phys. Rev. Mat.* **2**, 104402 (2018)

PNR Sensitivity



A single unit cell with a net magnetization of 40 emu/cc

PNR Sensitivity



$SrRuO_3$ (1 u.c.)/$SrTiO_3$ (3 u.c.)

Z. Cui, *Science Advances* **6**, eaay0114 (2020)