

# Nanomagnetism

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Oxford School of Neutron Scattering

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Years of ISIS Neutron  
and Muon Source



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# What this will be about?

- Housekeeping: Assumptions, Me, acknowledgements
- Motivation: Why bother with neutrons for magnetism.
- NR refresher.
- PNR examples.
- PA examples.
- 2 SANS examples.

# Some Assumptions:

- Assumption 1: You made the lectures (I managed this one 100% on the 2005 OSNS 19 years ago)
  - Specifically, you were in Nina's Talk on NR/SANS?
  - Specifically, you were in Ross Stewart's Lecture on Polarised Neutrons?
- Assumption 2:
  - You were awake (maybe I managed to be awake like 60% of the time)
- Assumption 3:
  - You were paying attention ( ok 30-40%)
- Assumption 4 :
  - You learned something... (20% Honest, I was on the winning pub quiz team that year which I take as proof of this)

**Surely you can beat me on this!**



OSNS 2005

# Who am I?

- Christy Kinane
- Instrument scientist working on the POLREF Polarised Reflectometer (NR/PNR/PA) at ISIS.
- **Hence this talk will be NR/PNR/PA heavy.**
- Work mainly on magnetic thin films and superconductors.
- If you have any questions, please contact me on:  
[christy.kinane@stfc.ac.uk](mailto:christy.kinane@stfc.ac.uk)
- Or we can go through things in the tutorial later.



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[www.isis.stfc.ac.uk](http://www.isis.stfc.ac.uk)

[@isisneutronmuon](https://twitter.com/isisneutronmuon)

[uk.linkedin.com/showcase/isis-neutron-and-muon-source](https://uk.linkedin.com/showcase/isis-neutron-and-muon-source)

## Acknowledgements: (People I have stolen stuff from after asking permission)

Andrew Caruana, ISIS

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John Webster, ISIS

Max Skoda, ISIS

Groan Nilsen, ISIS (Polarised neutron human)

Ross Stewart, ISIS (Very Polarised neutron human)

Diego Alba-Venero, ISIS (HCM SANS human)

Dirk Honecker, ISIS (HCM SANS human)



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Julie Borchers NCNR, NIST

Alex Grutter NCNR, NIST

Purnima Balakrishnan, NIST



Nina Juliane- Steinke, ILL



# What is Nanomagnetism?

## ***Colloquium: Opportunities in nanomagnetism***

S. D. Bader

*Materials Science Division and Center for Nanoscale Materials, Argonne National Laboratory, Argonne, Illinois 60439, USA*

(Published 3 January 2006)

Nanomagnetism is the discipline dealing with magnetic phenomena specific to structures having dimensions in the submicron range. This Colloquium addresses the challenges and scientific problems in this emerging area, including its fabrication strategies, and describes experiments that explore new spin-related behaviors in metallic systems as well as theoretical efforts to understand the observed phenomena. As a subfield of nanoscience, nanomagnetism shares many of the same basic organizing



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S.D.Bader, REVIEWS OF MODERN PHYSICS, VOLUME 78, JANUARY 2006

# Grand Challenges: Nanomagnetism



# So what is a large-scale structure?

- Well that depends on who you talk to!



The extremes



Terribly big and really old!!

Units of billions of years and  
Giga light years. So  
effectively unmeasurable!

Knee high to a grasshopper and  
very short lived!

$10^{-15}$  m and smaller down to the  
plank time and length. So  
effectively unmeasurable!

The bizarre thing here is that at either end of  
the scale things start to become  
indistinguishable and look the same. That's  
the problem with space it's both mind boggling  
big and really really tiny.

# What is a large-scale structure?



We mean  $10^{-10}$  m to 0.1m  
and  $10^{-9}$ s to 10s of seconds

## Actual Everyday Materials!

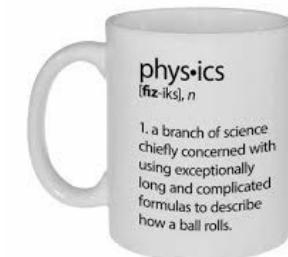
(Also known as where proper real science happens only without Brian Cox (Besides Jim Al Khalili is clearly the thinking man or woman's Brian Cox.)



My Cat/Monsters  
(Biology)



Beer  
(Chemistry)



Tea!  
(Physics)



This is a  
hitchhiker's  
guide to the  
Galaxy  
reference



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Note: My cat thinks she is the Universe and is more than willing to try and communicate this to you at 4am in the morning for no apparent reason, least you forget.

# Motivation: why neutrons?

- The design of new magnetic materials and devices requires a detailed microscopic understanding of their mechanisms and properties.
- Neutrons have a magnetic moment, and suitable wavelengths and energies to investigate a range of phenomena:

The three panels are arranged horizontally under a bracket that spans all three sections.

- Skymions**: A 3D visualization of a skyrmion lattice, showing a circular arrangement of small magnetic vortices with arrows indicating their orientation.
- Spin Seebeck effect**:
  - a Thermocouple**: Shows two different metals, Metal A and Metal B, connected by a thermocouple. A temperature gradient  $\nabla T$  is applied between them, with heat flow indicated by red arrows. Electromotive forces  $E$  are generated at each junction, which are measured by a voltmeter  $V$ .
  - b Spin Seebeck effect**: Shows a metallic magnet with a temperature gradient  $\nabla T$  and a resulting spin current  $\mu_\uparrow - \mu_\downarrow$ .
- Novel spintronics**: A diagram of a heterostructure device. It shows a Fermi surface ( $E_F$ ) in a circular inset, a source contact  $S$ , and a ferromagnetic metal (FM) layer. The device is composed of  $Bi_2Se_3$  layers. Arrows indicate electron flow and magnetic fields.

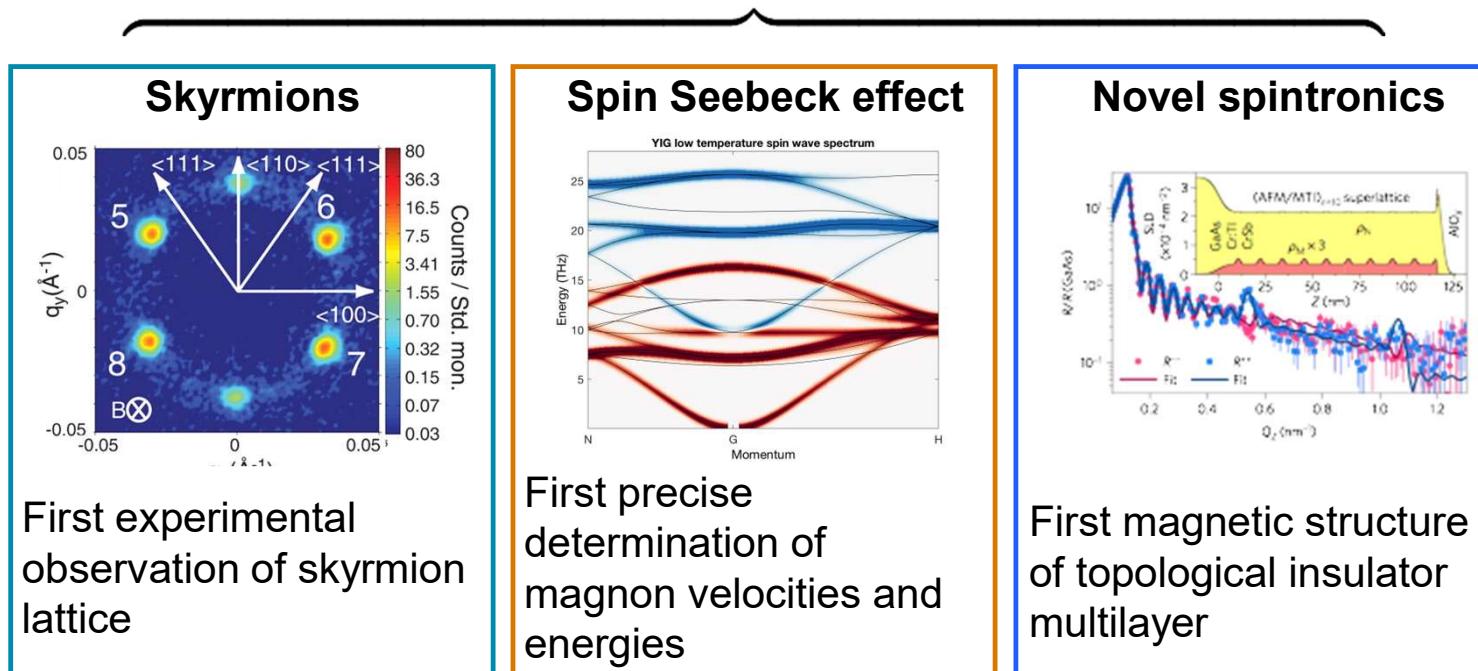
**First experimental observation of skyrmion lattice**

**First precise determination of magnon velocities and energies**

**First magnetic structure of topological insulator multilayer**

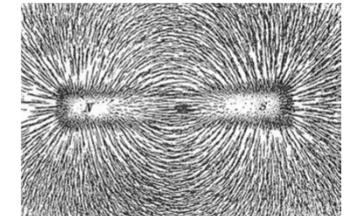
# Motivation: why neutrons?

- The design of new magnetic materials and devices requires a detailed microscopic understanding of their mechanisms and properties.
- But, neutrons are hard to produce and focus, so real space techniques are not viable. Need to work in reciprocal space.



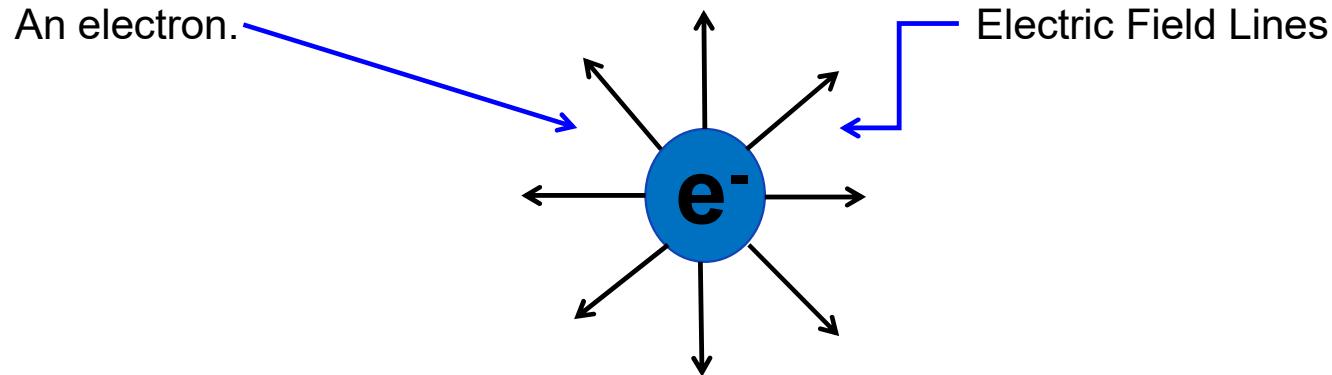
# Magnetism – History

- 800 BC/BCE approx: Magnetism has been known to humans for almost 3000 years (reported in Greek literature by the year 800 BC/BCE.
  - Magnetite ( $\text{Fe}_3\text{O}_4$ ) or Lodestone (leading stone) was mined in Magnesia in ancient Greece.
- 200 CE/AD approx China: First magnetic technological application: the compass. China before 200 AD/CE
- 1269 - Pierre de Maricourt found that magnets have two poles
- 1600 - W. Gilbert published all his experiments on magnetism on *De Magnete*.
- 1820 - Oersted and Ampere discovered the connection between electricity and magnetism. They started the idea that magnetism is caused by internal electrical currents.
- 1845 - Faraday first used the term “*magnetic field*” .
- Magnetism can only partially be explained with classical (statistical mechanics) physics.
- A quantum mechanism is required for a more complete picture.



# What is Magnetism?

*Magnetism has its origin in electric currents and the fundamental electric properties of elementary particles.*



- Electric charge can be negative or positive (Electrons or Positrons, respectively).
- Field lines in theory stretch out to infinity.
- **Very important to note electric field lines are open not closed!!!!**
- Electric field travels at the speed of light.
- Known as an electric monopole. (As far as we know there are no magnetic monopoles.)

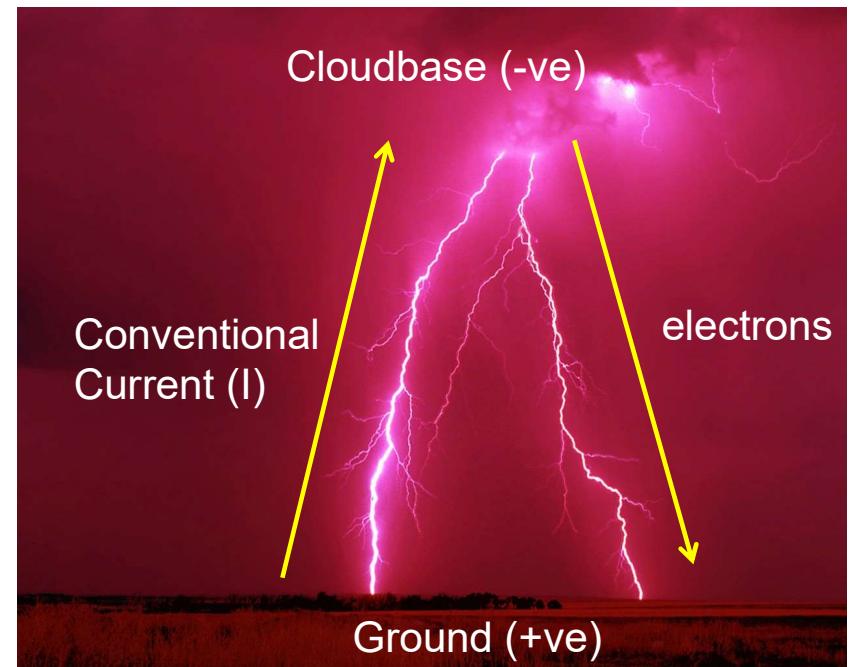


You can get  
fluffy neutrons!

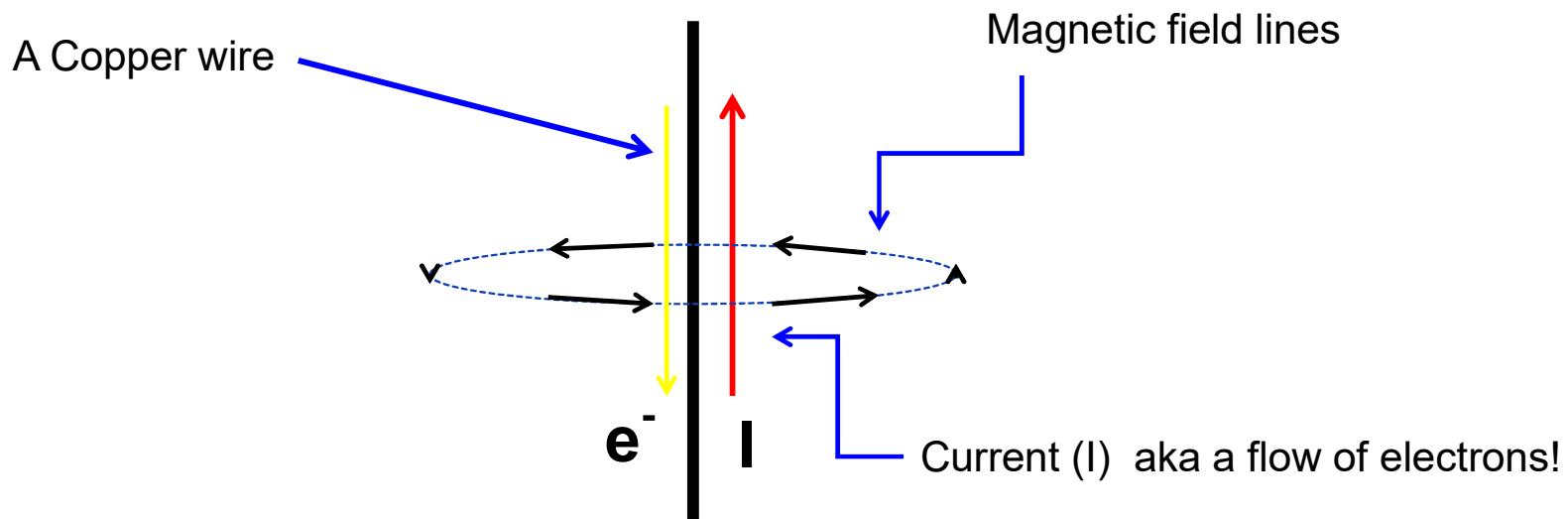


# So the current from a lightning bolt flows into the clouds.

- Conventional current always flows from positive to negative.
- In reality electrons flow from negative to positive.
- André-Marie Ampère is worth a lookup.



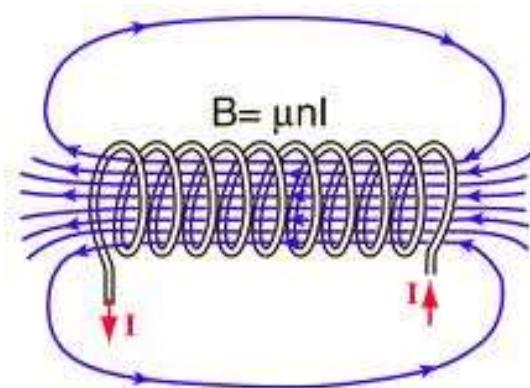
# Current flowing in a wire



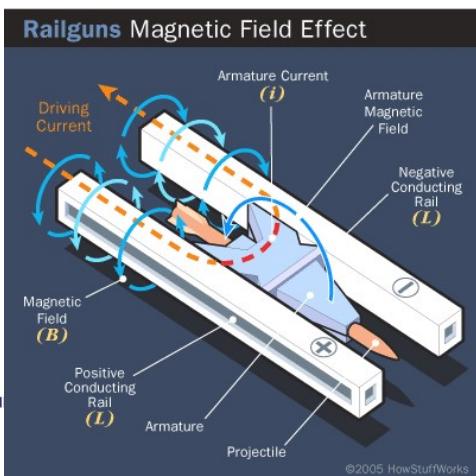
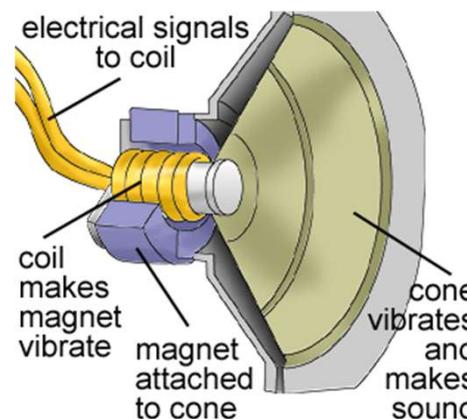
- Magnetic field lines are closed. They close back in on themselves.
- Electric current flowing in a wire generates a magnetic field. (via special relativity and length contraction!!!!)
- Check out this 5-minute video on how this works <https://www.youtube.com/watch?v=1TKSfAkWWN0>
- These circular field lines form concentric circles which stack out to an infinite distance.
- Magnetic force travels at the speed of light.
- **The famous right hand thumb rule.**

# Solenoid

- Basically a coil of wire!
- It is the basis of lots of technology from Faraday's time till present day!



The magnetic field is concentrated into a nearly uniform field in the center of a long solenoid. The field outside is weak and divergent.

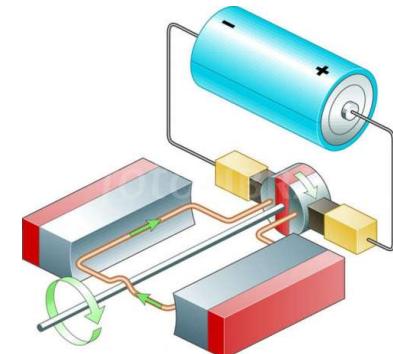
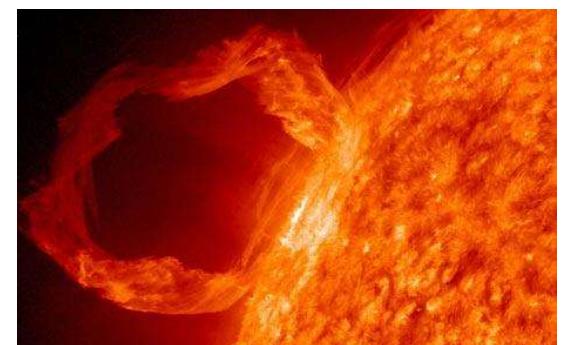
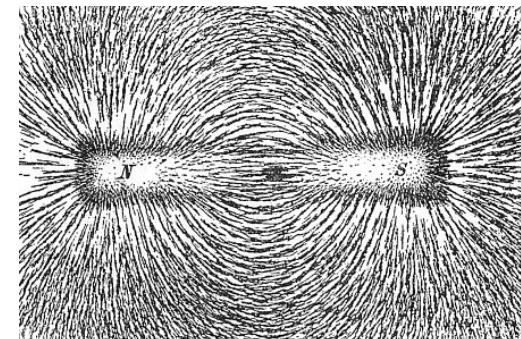


- Look up the USA's Star Wars program.
- Scarily BAE systems testing ship based rail gun today . (32 mega joules or 8Kg of TNT)
- Yes one was in the 2<sup>nd</sup> Transformers movie. (yes the film was rubbish.)



# ELECTROMAGNETISM!

- The basic links between magnetic fields and electric fields should now be clear.
- Magnetic fields are generated by moving electric charges.
- **Magnetic fields are dipolar in nature, while electric fields are monopolar in nature.**
- The size of magnetic fields is usually smaller than electric fields.
- Magnetic interactions follow field lines.
- Magnetic fields can interact with electric charges and vice versa as well as permanent magnets made of Ni, Fe, Co, Rare Earths or Alloys.
- This is the basis of electric motors and all electromagnetic technology.
- Look up the story of Thomas Edison and Nicola Tesla.

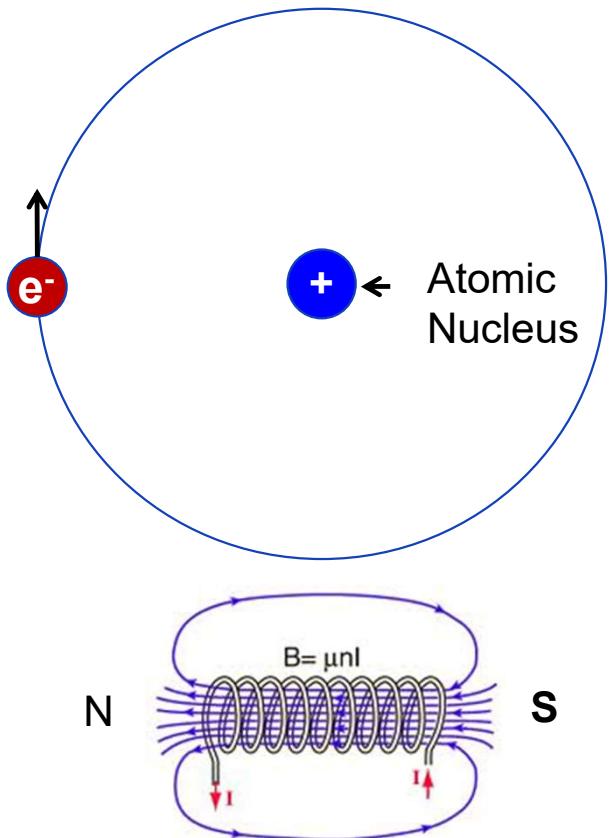




## Fridge Magnets (admittedly not a nanomagnet)

- To understand a fridge magnet, we must enter the world of the physics of solids, referred to as the Solid State or Condensed Matter by physicists,
- There are two basic sources of magnetism:
  - Orbital angular momentum
  - Spin.

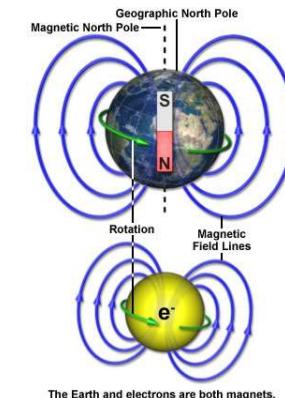
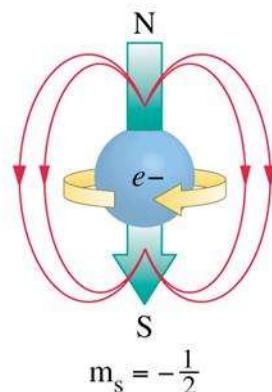
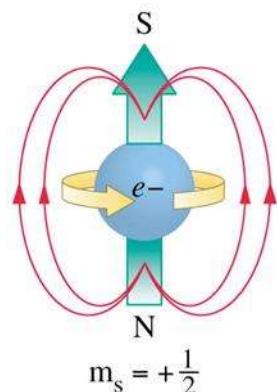
# Orbital angular momentum



- Electrons like to hang around in pairs.
- Magnetism requires an unpaired electron.
- Electron orbits the nucleus forming a current loop.
- Classically this forms a small atomic solenoid which has similar field lines to a wire solenoid.
- This has a direction, the ends of which we label as North and South poles.
- This is called a magnetic dipole.
- Think spinning bicycle wheels!
- **However, this is a Classical approach and not correct.**

# Spin

- Elementary particles like electrons have a property called spin.



- "Spin" is a non-classical property of elementary particles, since classically the "spin angular momentum" of a material object is really just the total *orbital* angular momentum of the object's constituents about the rotation axis.
- Elementary particles are conceived as points, which have no axis to "spin" around, hence we are now firmly in the quantum universe where things are **Weird!**
- For simplicity think of the electron as a bar magnet.
- If you have two electrons then the spins cancel and you do not get any net magnetism.

# Ferromagnetism = Fridge Magnets

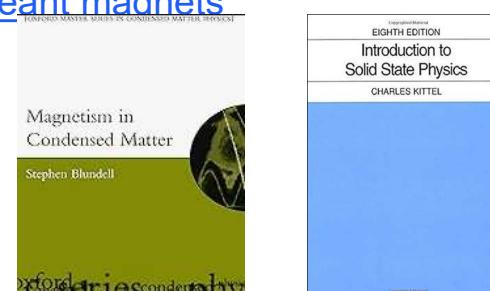
- All the magnetic atoms (e.g. "Fe") can talk to each other.
- This is via an exchange interaction.
- There are lots of different types of these interactions and they are very very important. However we are not going to talk about them as we don't have the time.
- Magnetic atoms, being friendly individuals, like to group together and point in the same direction. This is called a magnetic domain.
- Sadly like groups of people they often don't talk to other groups, so don't point in the same direction as the other magnetic domains.
- Normally the magnetic fields/ field lines of all the domains cancel out.
- **Hence why any old lump of iron does not immediately act as a magnet.**
- The lump of Iron has to be magnetised so that the domains all point in the same direction.
- [Check out this 6 minute long minutephysics explanation of permeant magnets](#)  
<https://www.youtube.com/watch?v=hFAOXdXZ5TM>
- We now have a fridge magnet!



Domains Before Magnetization



Domains After Magnetization



# Other types of magnetism

- **Paramagnetism/Diamagnetism.**
- Not that many uses in technology.
- Paramagnetism can be used to make fridges that get close to absolute zero.



- **Diamagnetism is exhibited by all materials to a lesser or greater extent.**
- It can be used to levitate things like frogs or light graphite wafers.
- Other forms of magnetism: Antiferromagnetism/Ferrimagnetism/Superparamagnetism.
- Check out Andre Geim of Nobel Prize fame for discovering Graphene.

# What kind of scientific information can be obtained from Neutron Reflectivity (NR)?

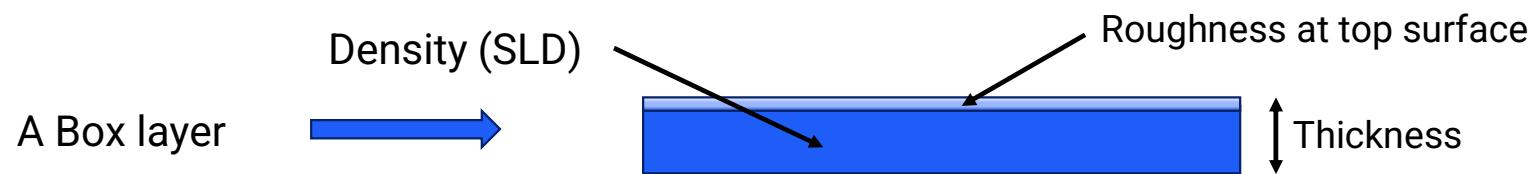
Specular Reflectivity (non-polarised) provides the chemical (isotopic) scattering length density (SLD) depth profile along the surface normal with a spatial resolution approaching half a nanometer (nm).

1. From basic theory of reflectivity, The SLD can be made using simple box models then requires 3 parameters:

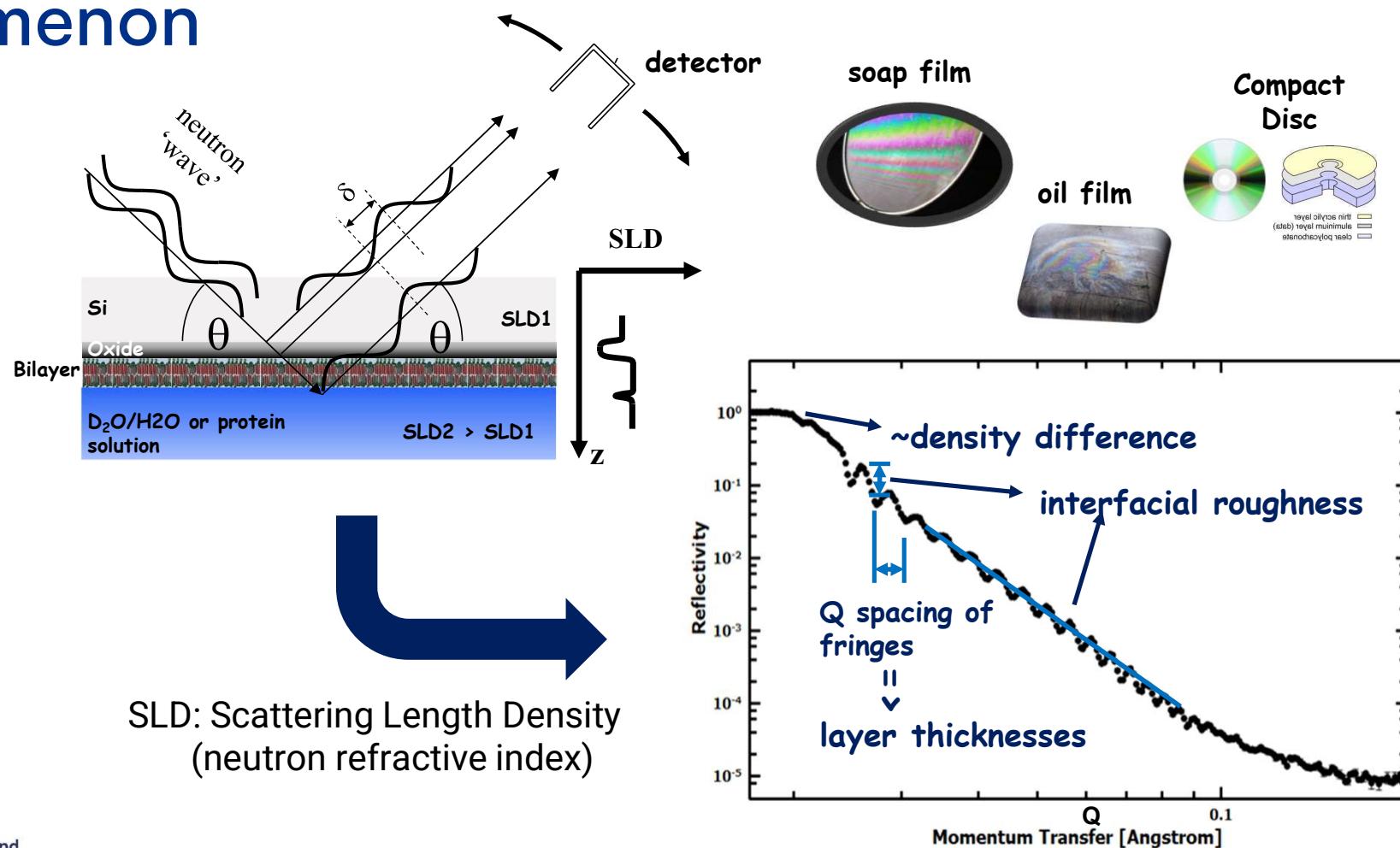
=> essentially thickness, roughness, density (SLD).

2. Scientific meanings of the parameters:

- a) **Thickness:** thermal expansion/Contraction, glass transitions, surface adsorption/desorption, kinetics, etc.
- b) **Roughness:** polymer reptation, interdiffusion, diffusion coefficients, surface tension, strain, etc.
- c) **Density:** Density variation, surface enrichment, surface segregation, Level of hydration, etc.



# Neutron Reflectivity - an interference phenomenon

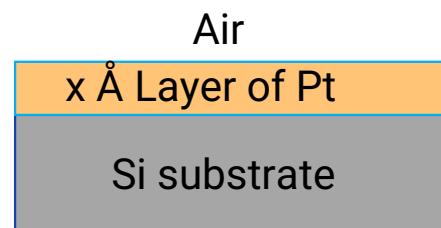
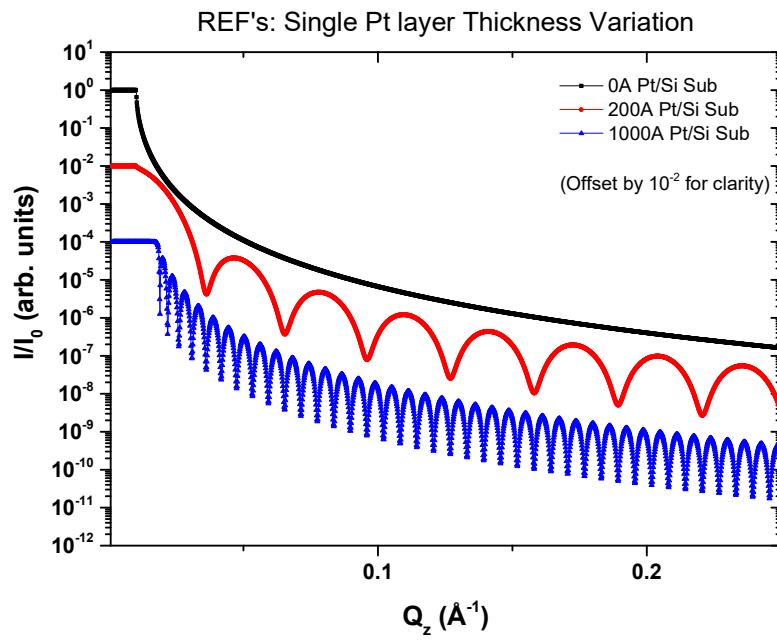


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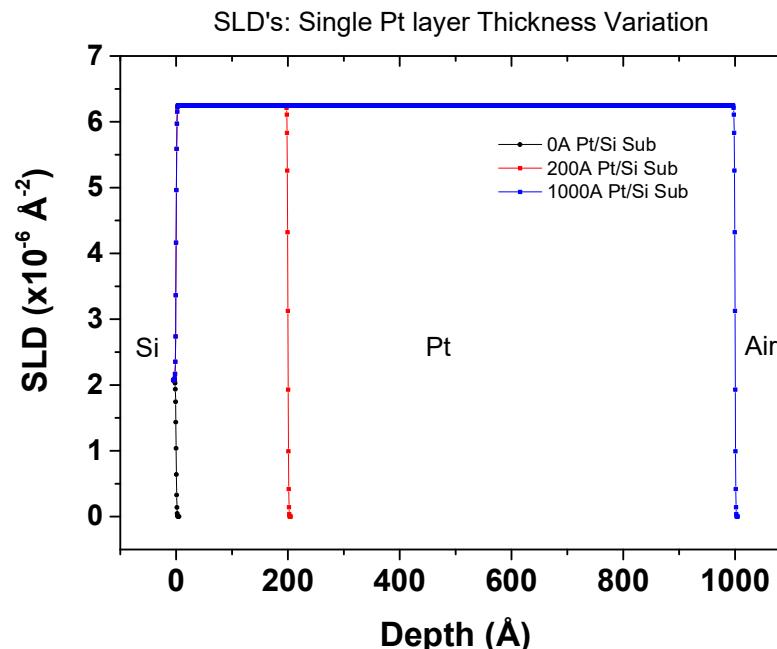
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- Logarithmic X axes should for a smooth sample give a linear die off for the intensity. This should match a  $1/Q^4$

# Thickness (t or d)



Where  $x = 0, 200$   
and  $1000 \text{\AA}$ .

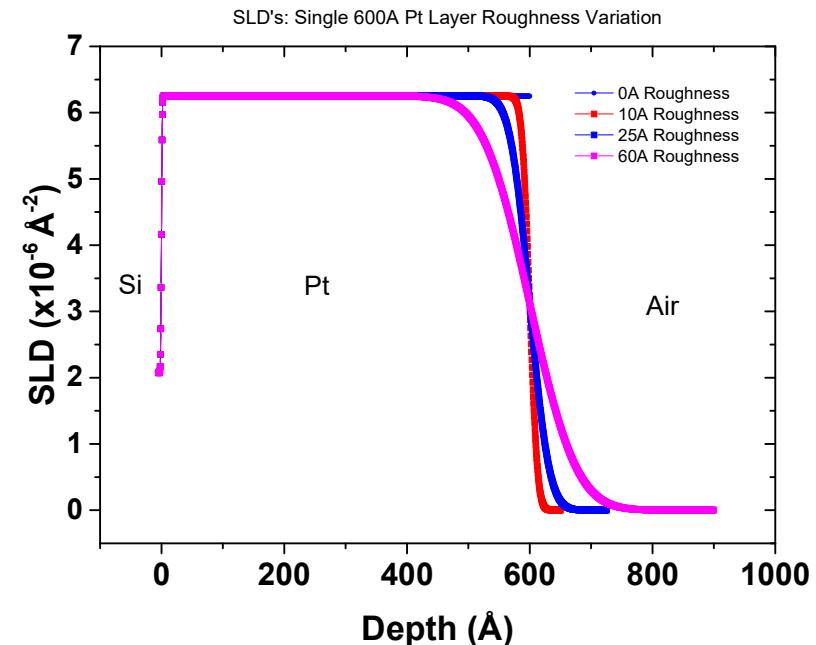
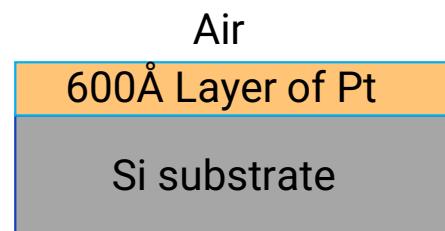
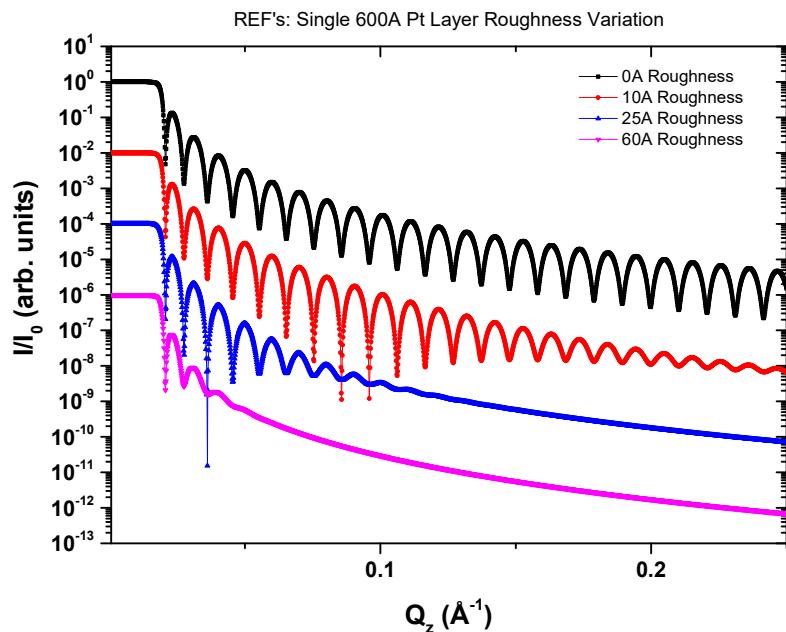


- Resolution is infinitely good in these simulations.
- Thin layers will appear at high Q.
- Thick layers will appear at low Q.
- This can greatly effect your count times!

- For a smooth sample with a linear X axis, the intensity should scale as  $Q^{-4}$  or  $\theta^{-4}$ .
- If there is no roughness applied this will be a straight line on a log/log plot.

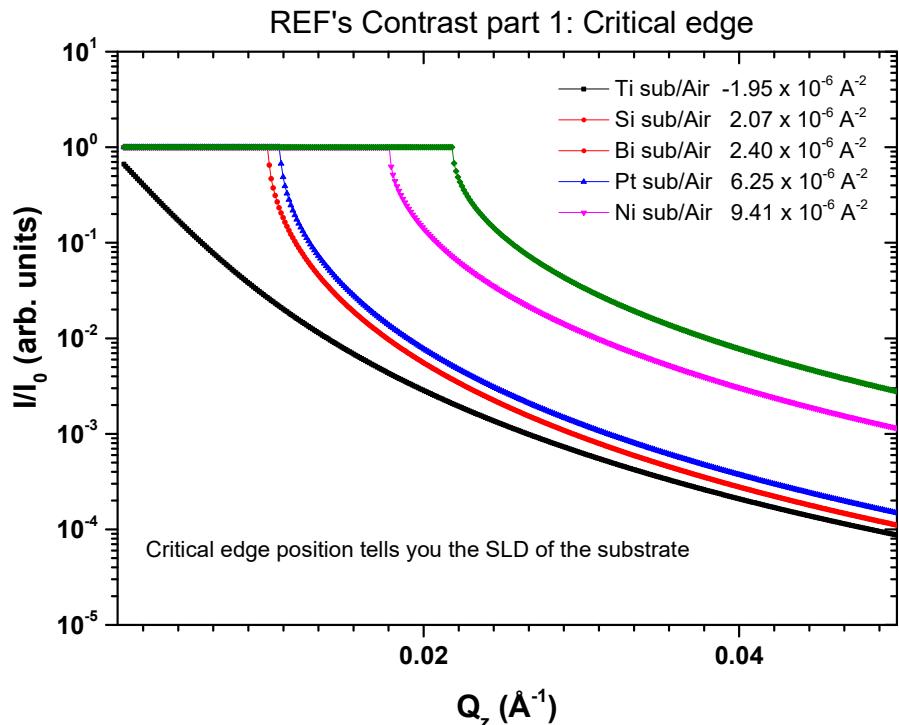
H. Kiessig Ann Phys 1931, 10, 769-788

# Roughness ( $\sigma_r$ )



- Roughness modelled as a smoothing of the SLD profile.
- Grading/interdiffusion also produces the same effect on the SLD as roughness. It requires off-specular scattering to differentiate between them.
- Note a small amount of roughness 60Å almost wipes out the reflectivity completely.

# Contrast Part 1: Substrate/Air Interface



$$Q_c = \sqrt{16\pi Nb} \quad \text{or more generally,}$$
$$Q_c = \sqrt{16\pi(Nb_1 - Nb_2)}$$

Where:

$Q_c$  = Critical Q

$N$  = number density (atoms/ $\text{\AA}^3$ )

$b$  = Scattering Length ( $\text{fm } 10^{-15}\text{m}$ )

$Nb$  = Scattering Length Density (SLD in  $\text{\AA}^{-2}$ )

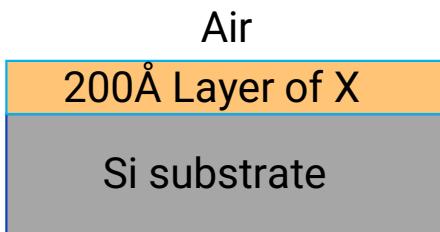
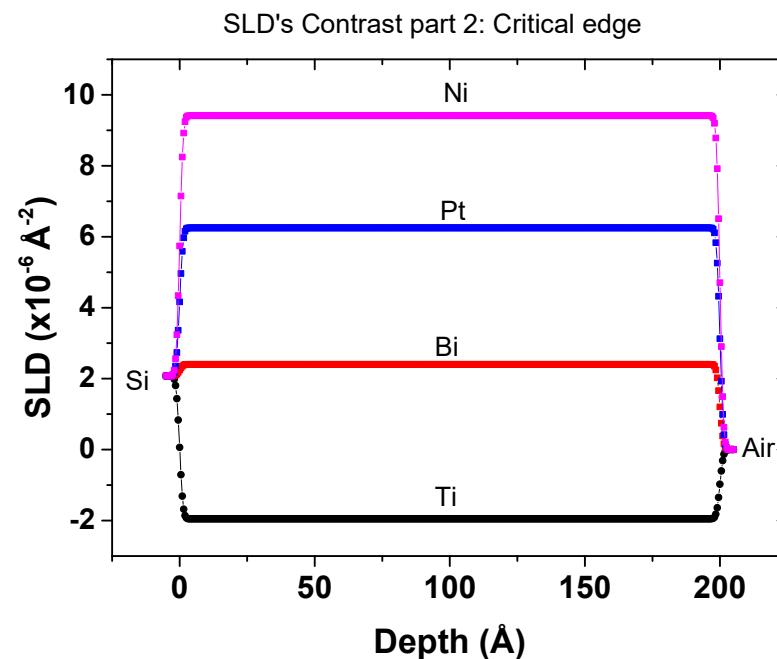
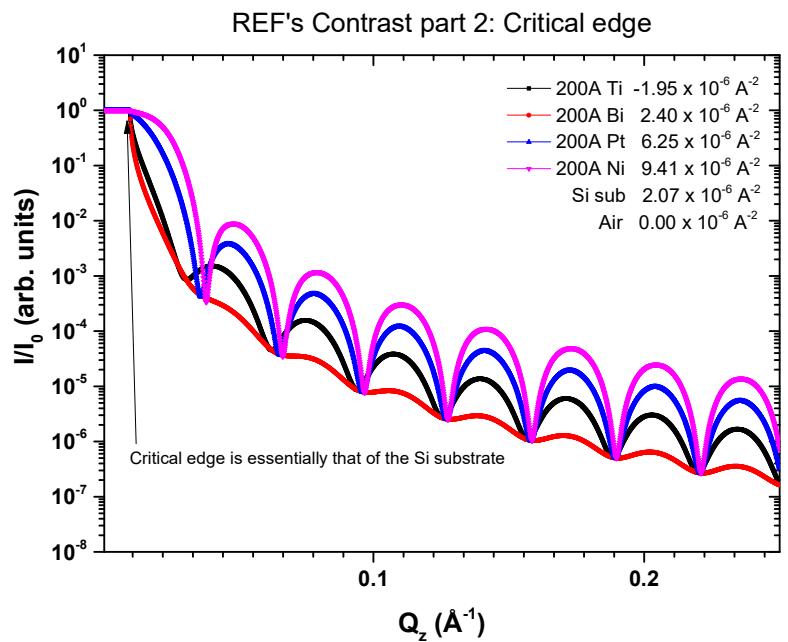
- Note the shift to higher Q as the SLD increases.
- Ti has a negative SLD, hence no critical edge.
- The critical edge position is normally given by the system components with the biggest relative SLD difference. Normally the substrate (subphase) vs the air (superphase).

Air (superphase),  $Nb_2$

Substrate X  
(Subphase),  $Nb_1$

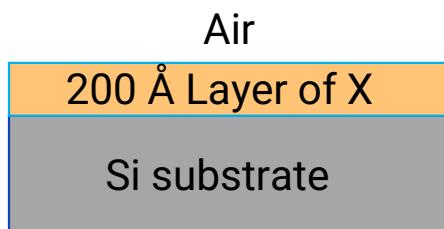
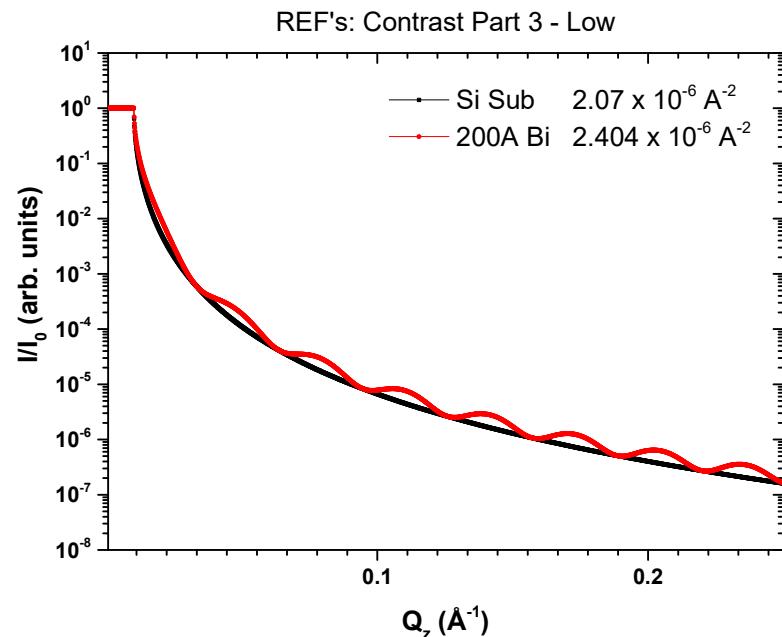
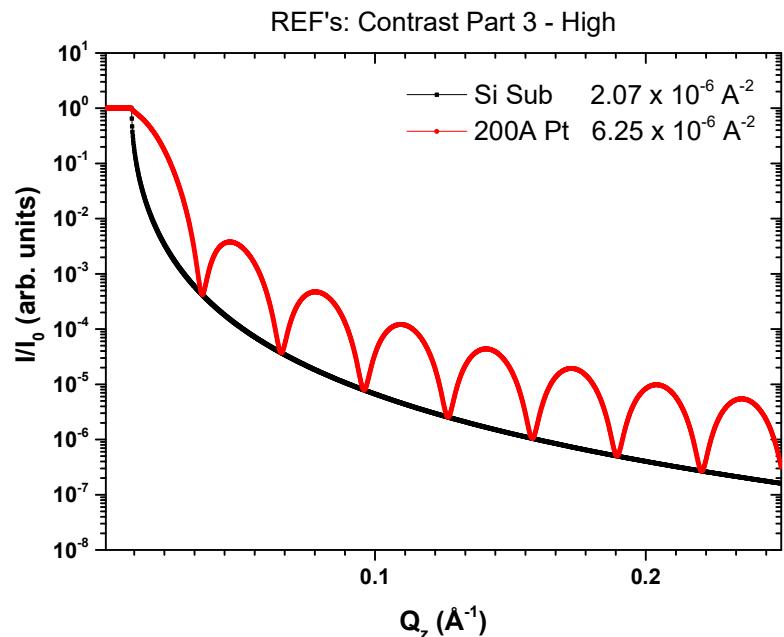
Where X can be any of Ti, Si, Bi, Pt or Ni.

# Contrast Part 2: Si(sub)/Layer(200Å)/Air



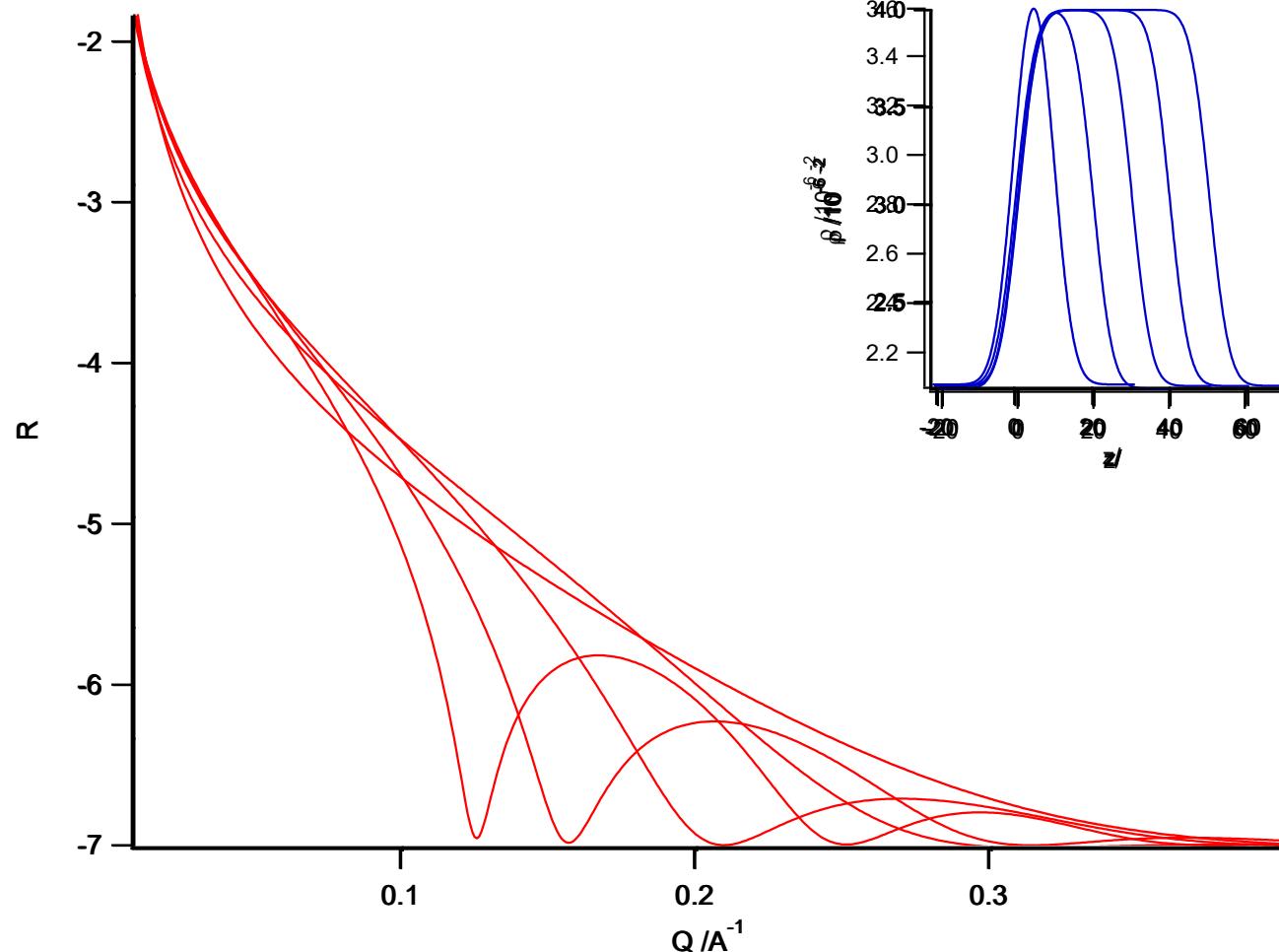
- Where X can be any of Ti, Bi, Pt or Ni.
- The height of the fringes is informative on the relative contrast of the layer to the substrate.
- The roughness is set to zero in all these cases.

# Contrast Part 3: Si(sub)/Layer(200Å)/Air



- Where X is either Bi or Pt.
- The substrate reflectivity should mark the bottom of the fringes

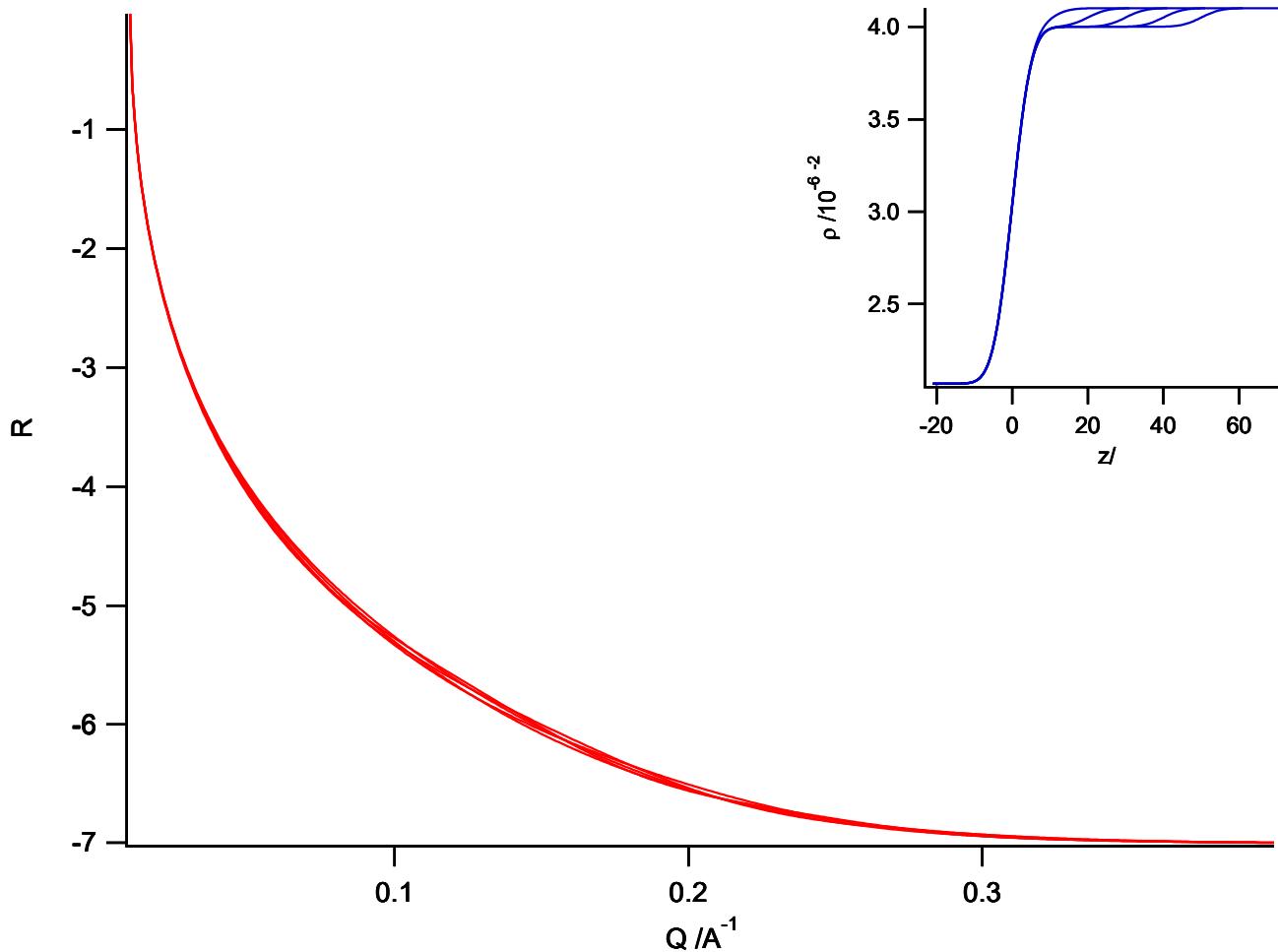
# 'Good' Contrast



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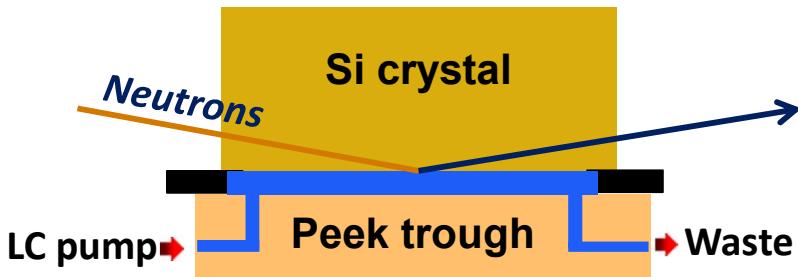
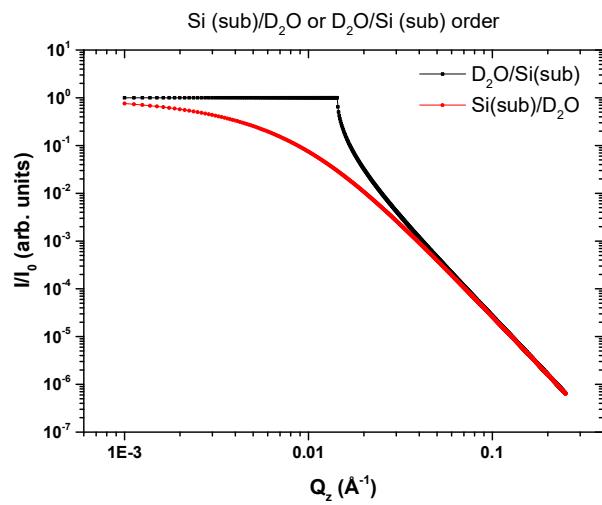
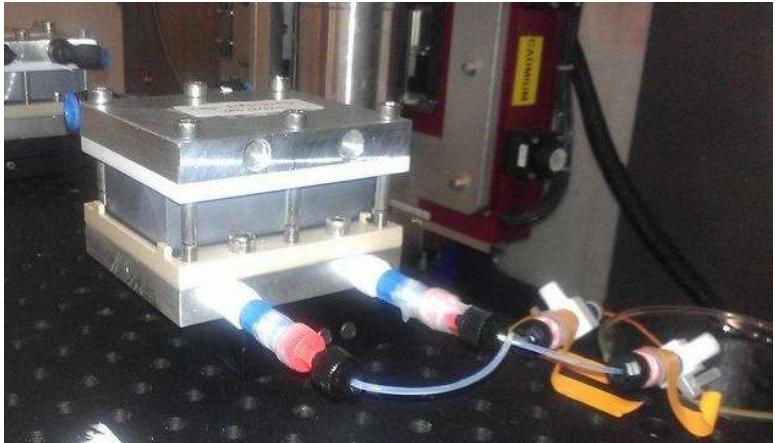
# 'Poor' Contrast



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## Contrast Part 4: The order can be important!!!!!!

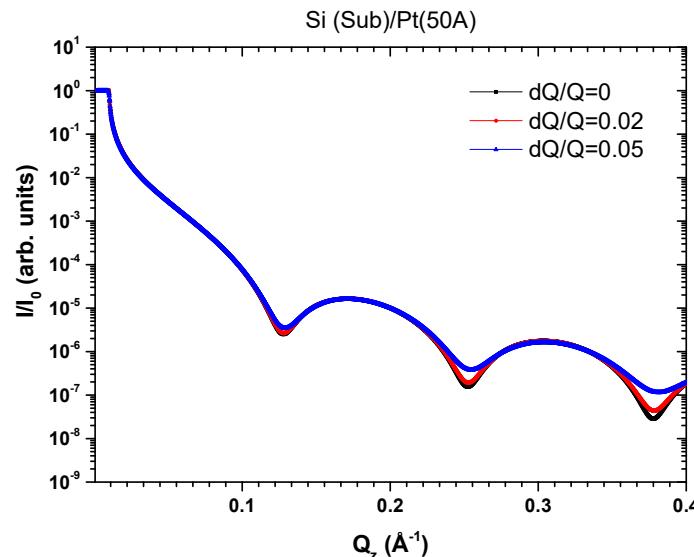
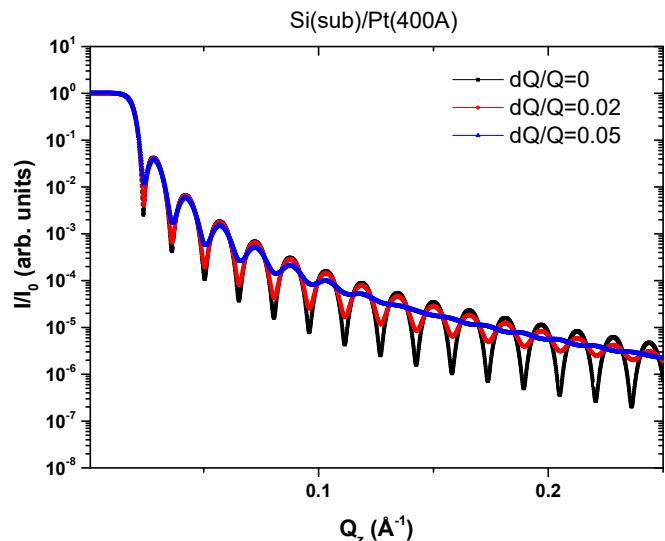


$$Q_c = \sqrt{16\pi(Nb_1 - Nb_2)}$$

- Air is not the only medium through which the beam can be passed.
- The order is important!
- Similar to refractive index.
- Contrast must be considered.
- Absorption must also be corrected for and incoherent background considered, when running and designing experiments.

# Contrast/Roughness and the perils of resolution

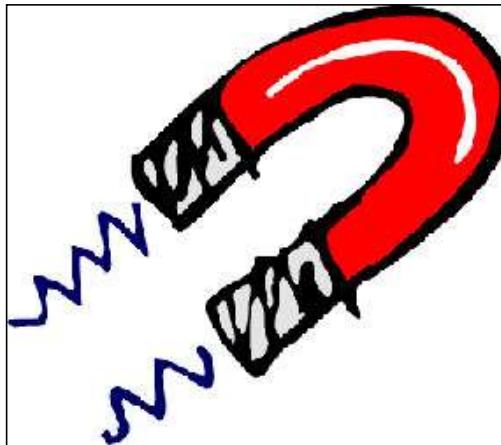
Resolution issues can look like contrast and Roughness!



- **Resolution damps interference fringes and rounds off critical edges (as does absorption).**
- Make an effort to know what the resolution you used in your experiment.
- Keep in mind that Time of Flight measurements have constant  $dQ/Q$  this is not the case for fixed slit monochromatic beamlines. Note. some Monochromatic beamlines dynamically open the slits to maintain a constant  $dQ/Q$ .
- If you are over illuminating your sample the resolution will be better than you think it is! **The sample can act as a slit!**
- This is not so critical for thin layers.

# Polarised Neutron Reflectometry (PNR)

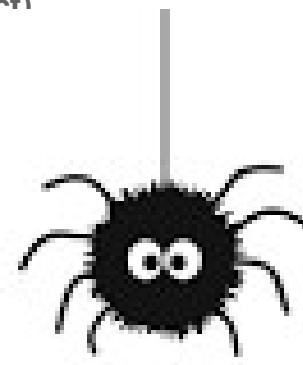
- NR measures the **nuclear** scattering length density profile (The Nuclear nSLD! It's very Important!).



- PNR measures the **magnetic** scattering length density profile. (The Magnetic mSLD)

# What kind of scientific information can be obtained PNR:

- Magnetometry (SQUID, VSM, MOKE):
    - Measure the bulk magnetic response of a sample
    - No spatial information
  - Electrical Transport:
    - Measures the conductive layers preferentially
    - Also no spatial information so very hard to interpret results beyond bulk response
  - Magnetic X-ray techniques (XMCD, XAS, XMLD):
    - Element specific, very high sensitivity.
    - Results hard to interpret! (Spin-Photon interaction indirect)
    - Light elements are difficult to measure.
    - Soft x-rays highly absorbing.
  - Microscopy (Electron, MOKE based, X-ray)
    - Surface sensitive only.
    - Sample environment limited.
  - Low Energy Muons:
    - Poor depth sensitivity.
    - Difficulties large internal magnetic fields.
    - Fantastic sensitivity to very small magnetic moments
- PNR:
    - Highly penetrating so can probe large volume. Can probe buried interfaces.
    - Spin Neutron interaction direct. Results easy to interpret.
    - Strong magnetic scattering
    - Contrast variation across the periodic table means light element easily measurable.
    - Isotope contrast variations available
    - Depth dependent magnetometer
    - Absolute moment
    - Vector magnetometer (in the plane of the sample)
    - Long coherence length



**PNR is an excellent tool to connect all these together!**

# What kind of PRACTICAL scientific information can be obtained PNR:

**Polarised Specular Reflectivity provides both the chemical/nuclear (isotopic) and the Magnetic scattering length density depth profile along the surface normal with a spatial resolution approaching half a nanometer (nm).**

1. In NR you get three basic parameters assuming a box model is used to construct the SLD profile:

=> essentially thickness, roughness, density (nSLD).

2. In PNR these are joined by three more magnetic parameters:

=> essentially magnetic thickness, magnetic roughness and magentic density (mSLD).

- a) **Magnetic thickness:** Magnetic dead layers, magnetic proximity effects, topological insulators.
- b) **Magnetic roughness:** Canting, spirals, coupling, superconducting vortices.
- c) **Magnetic Scattering Length Density:** Total moment, interlayer coupling (RKKY AF coupled layers), inhomogeneities, magnetic transitions (AF/FM/P).

- Note: PNR is NOT sensitive to inter-atomic magnetic order like antiferromagnetism!

# Properties of Hysteresis loops (Terminology)

- Field ( $H$ ) and Moment ( $M$ )  
SQUID, VSM (PNR/PA!)

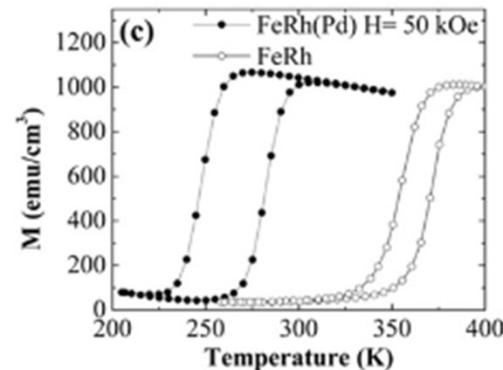
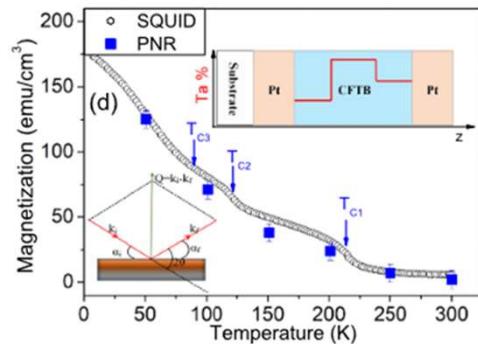


- Relative response  
to Field ( $H$ ) only

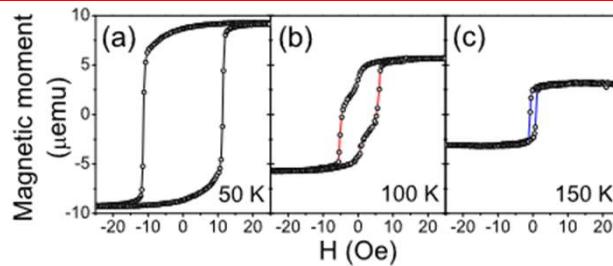
MOKE, XMCD



- Magnetisation vs Temperature - ( $M$ vsT)



- Magnetisation vs Applied Field - ( $M$ vsH)



- The applied field and thermal histories are very important in magnetic materials.

- C. J. Kinane *et al.* New Journal of Physics 16 (2014) 113073
- O Inyang *et al.*, PRB 100, 174418 (2019)

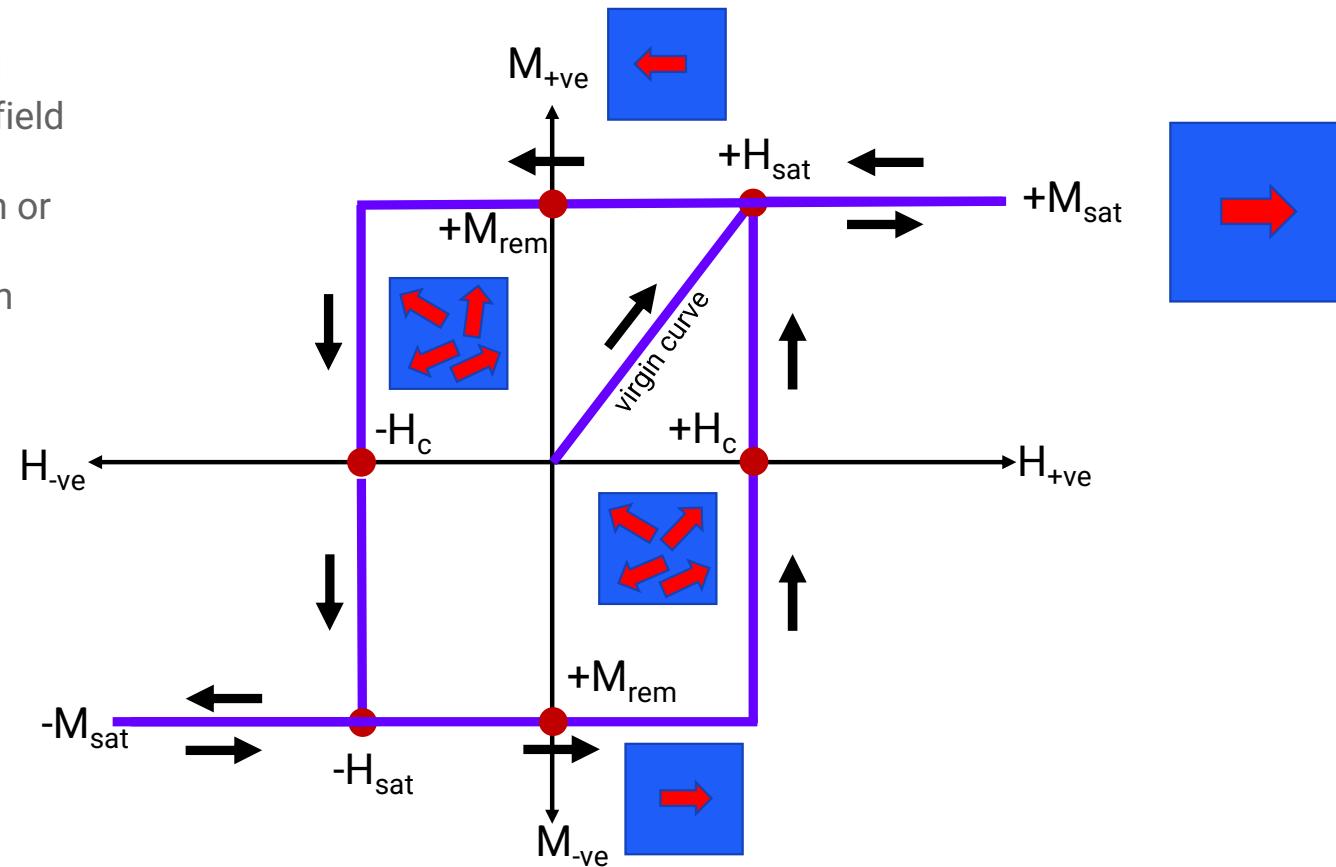
# Properties of Hysteresis loops (Terminology): Magnetic Hysteresis

$H_c$  = Coercivity or coercive field

$H_{\text{Sat}}$  = Saturation or saturation field

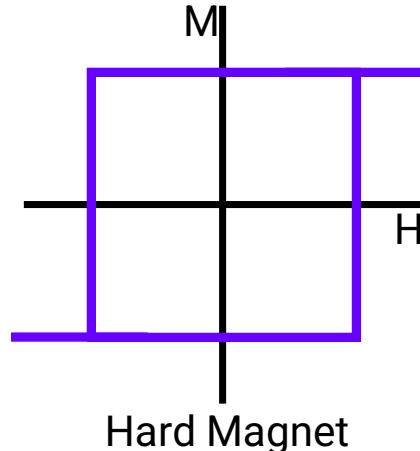
$M_{\text{Rem}}$  = Remnant magnetisation or retentivity.

$M_{\text{sat}}$  = Saturation magnetisation

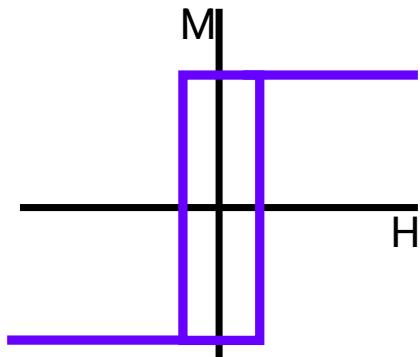


- The properties of a magnetic hysteresis loop are often thought of as scalar in nature (directionless) but in fact are vectorial. They apply to the direction the  $H$  field is applied in the sample.
- Hysteresis means the magnetic history of the sample is VERY important!

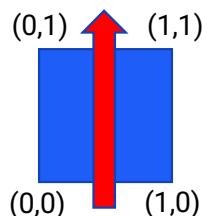
# Properties of Hysteresis loops (Terminology):



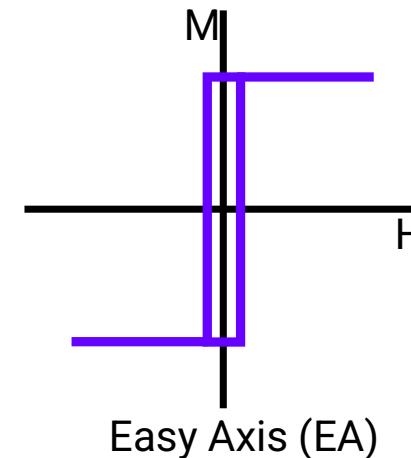
Hard Magnet



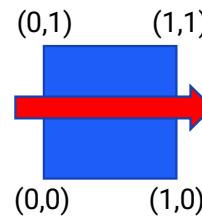
Soft Magnet



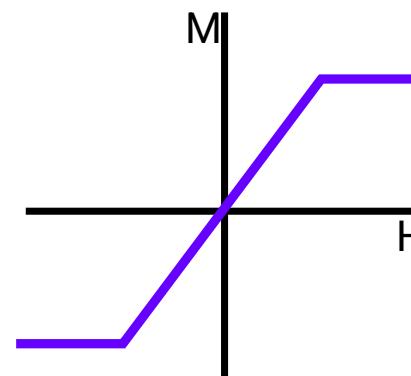
$H$  field applied in the  $(0,1)$  direction



Easy Axis (EA)



$H$  field applied in the  $(1,0)$  direction

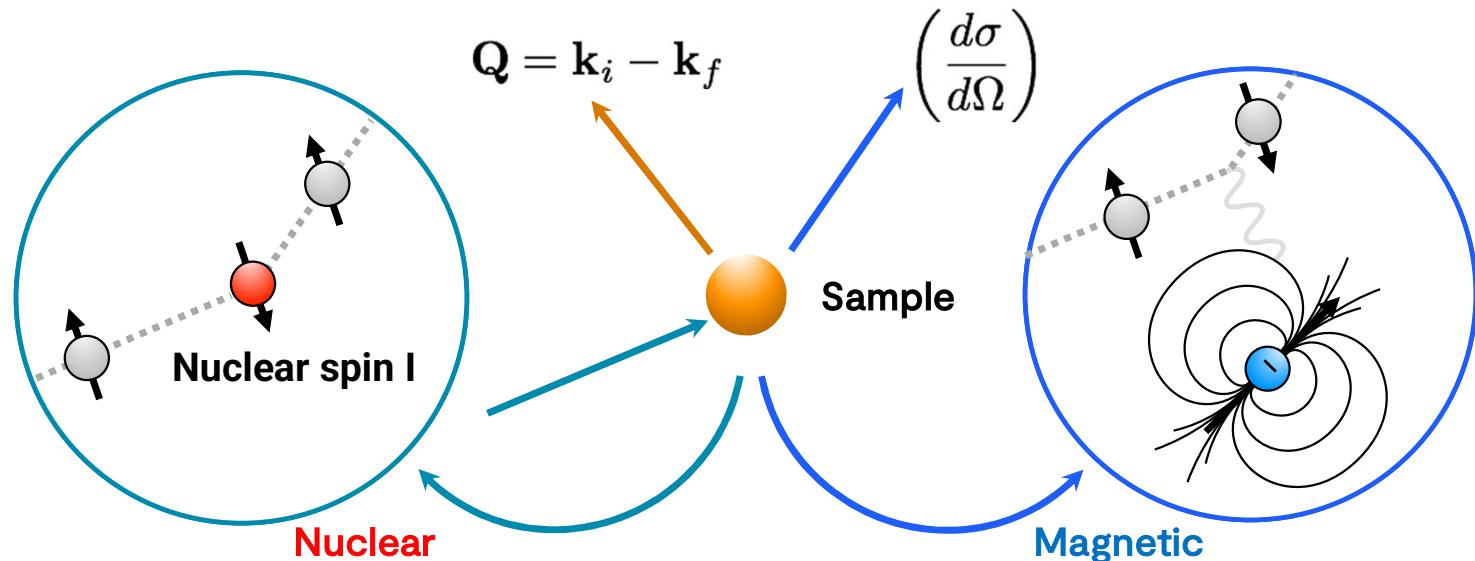


Hard Axis (HA)

- Anisotropy has many forms – Magnetocrystalline, shape etc
- The direction that the  $H$  field is applied affects the values of  $H_c$ ,  $H_{sat}$ ,  $M_{rem}$ ,  $M_{sat}$
- it is very important to know the sample orientation vs the magnetic field!

# Neutron-electron interaction

The neutron has magnetic moment which can interact with sample moments:



Interaction is between dipolar fields of neutron and unpaired electron(s) → directional dependence.

Neutrons scatter magnetically for the B field of the magnetic material!

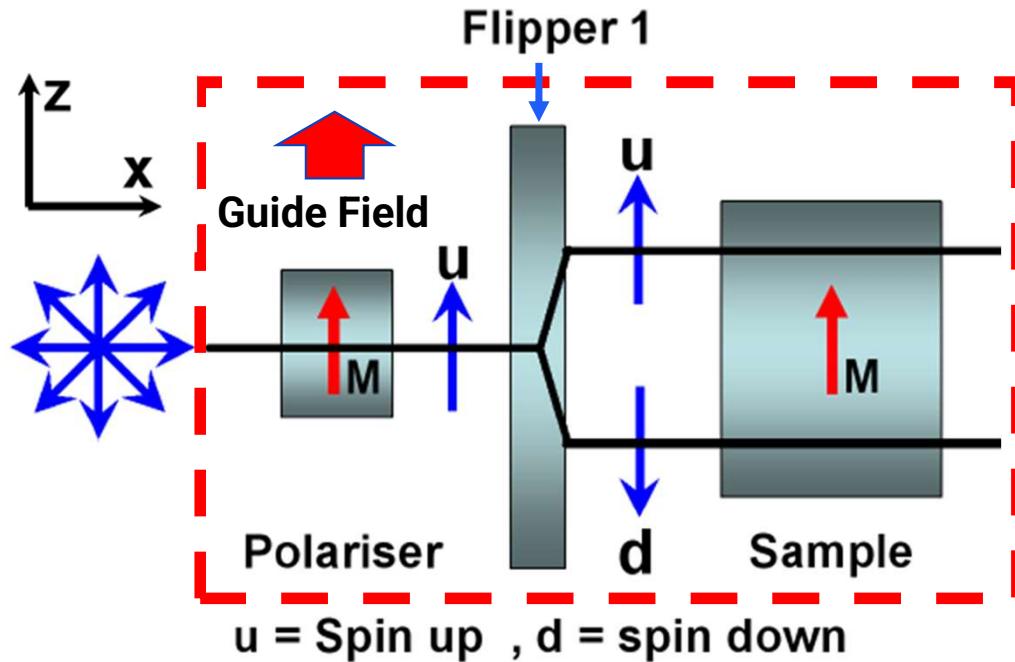
Strength of magnetic interaction similar to that neutron and nucleus (unlike X-rays).

A neutron is a spin  $\frac{1}{2}$  particle with a magnetic dipole moment, effectively it's a little bar magnet. (like a fridge magnet only smaller)

Thanks to G Nilsen for this slide

# Polarised Neutrons PNR or Half Polarised:

Unpolarised neutrons have no orientation



Now measure two reflectivity curves:  
i) Spin up  
ii) Spin down.

Experiments now takes 4 times as long to get similar statistics!

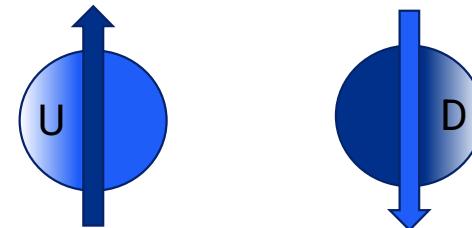
- There are several ways of polarising and flipping neutrons, I direct you to Ross Stewart and Nina Juliane Steinke's lectures for more details.
- It is the difference between the reflectivity curves of the two spin states that allow the magnetism to be probed.

- W. Gavin Williams Polarized neutrons Oxford Science
- A.-J. Dianoux et al, Neutron Data Booklet (Institut Laue-Langevin, 2002), 1st ed.

# PNR Terminology:

- In PNR we refer to measuring the spin states.
- These are referred to by a multitude of names but ultimately all the names are labels referring to the spin of the neutron being aligned “Parallel” or “Antiparallel” to the guide field. Labels include:

- Parallel => Up, U,  $I^+$ ,  $\uparrow$ , or just +
- Antiparallel => Down, D,  $I^-$ ,  $\downarrow$ , or just -



- It is important to note that in PNR the “Up” and “Down” states contain the Spin flip components as well. E.g. Up = UU + UD and Down = DD + DU but more on this later.
- Maintaining the guide field on a PNR beamline is VERY VERY important!
- The classic experiment of measuring the depolarisation of a spanner/Allen key on the guide field box has amazing stats and has been reproduced accurately tons of times now! We don’t need more data for it!!!!

# Polarised Neutron Reflectivity (PNR):

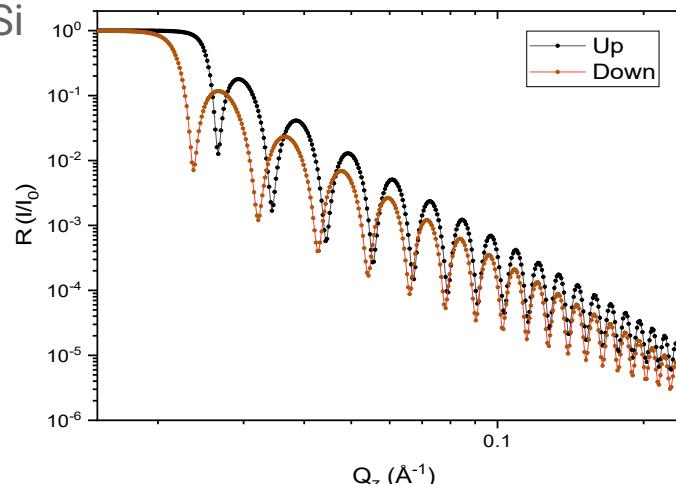
- It is assumed that the polarisation vector and magnetisation are parallel (We set the beamline up so this is as true as possible)

$$V = V_n \pm V_m \quad \text{where } V_n = \frac{2\pi\hbar^2}{m} Nb \text{ and } V_m = \frac{2\pi\hbar^2}{m} Np = \pm \mu_n B \quad \text{With } p = (2.695 \times 10^{-4}/\mu_B)|\mu_i|$$

For a single magnetic layer

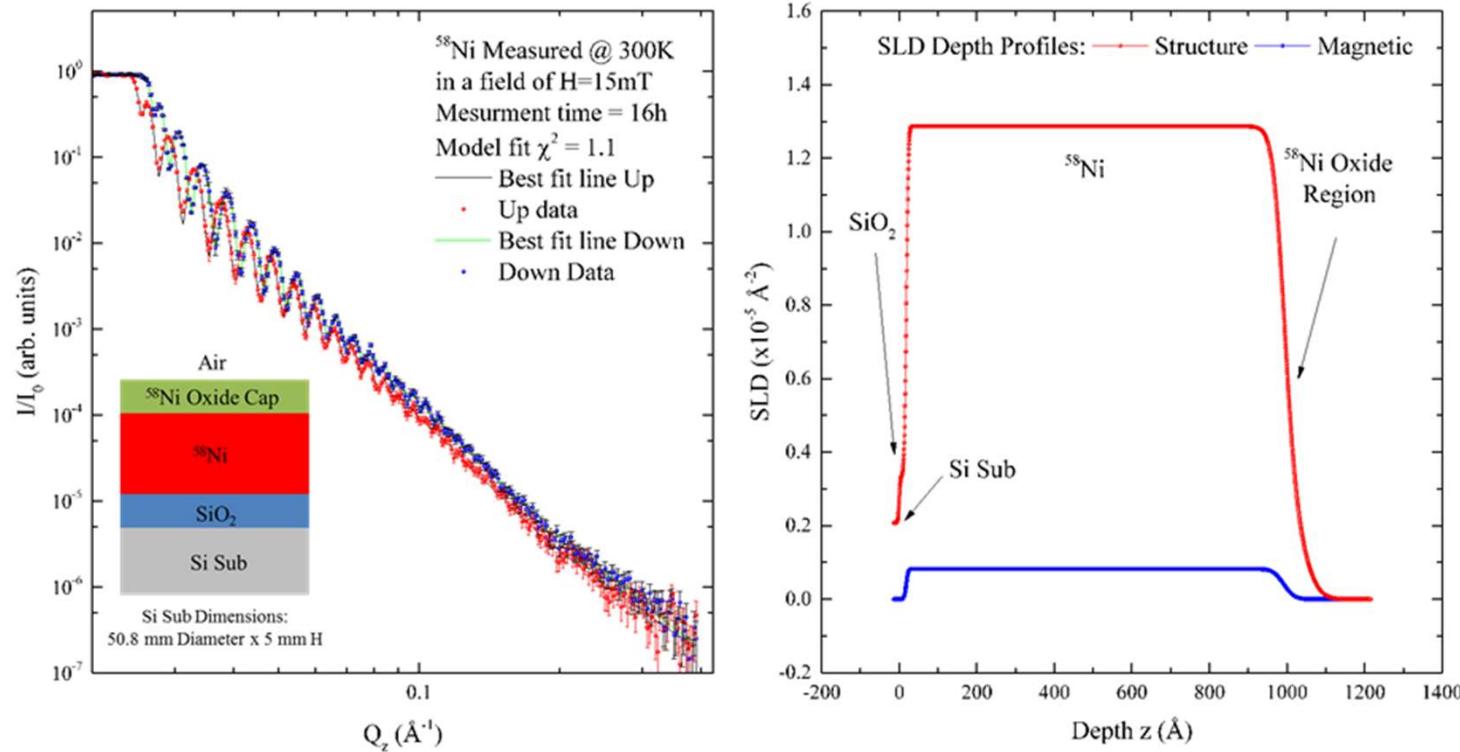
$$V = \frac{\hbar}{2\pi m} N(b_N \pm b_m)$$

- This essentially means you get two reflectivity curves as the magnetic layer has two different values for its SLD depending if M is parallel or anti-parallel to the polarisation  $\mathbf{P}$  direction established by the guide field.
- For example A 500 Å Ni layer on Si substrate



- Bland et al, Phys Rev B, 46, 3391 (1992)
- Zabel et al Physica B 276-278, 17 (2000)
- R. M. Moon et al Phys Rev, 1969, 181, 920-931
- S. Blundell et al, JMMM, 1993, 121, 185-188
- Bland et al, Phys Rev B, 46, 3391 (1992)
- G. L. Squires introduction to the Theory of Thermal neutron scattering
- Modern Techniques for Characterizing Magnetic Materials Edited by Yimei Zhu, Springer
- Neutron Scattering from Magnetic Materials, editor Tapan Chatterji, Elsevier

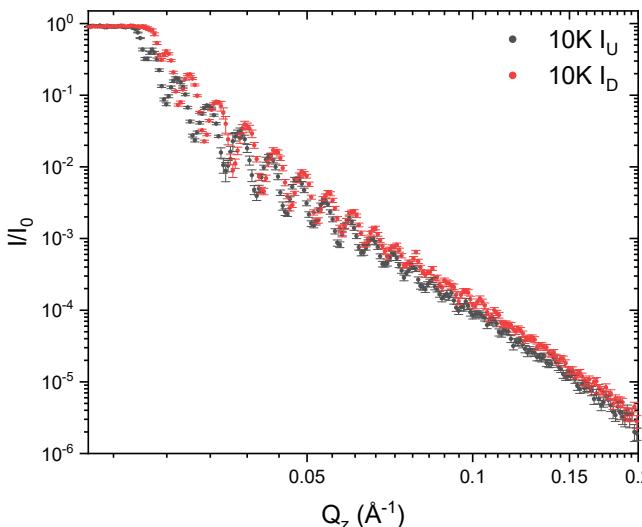
# PNR: An example of PNR from a simple Ni film.



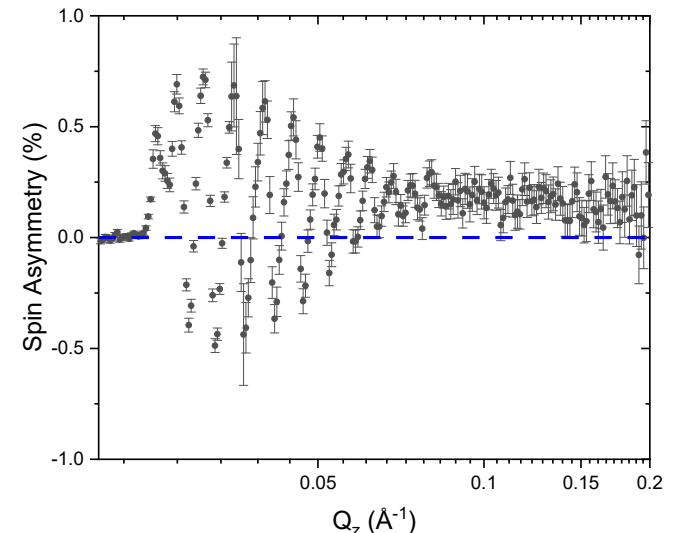
- PNR provides both the Nuclear (structural) and the magnetic SLD depth profile.
- Effectively functions as a depth dependent magnetometer
- But takes longer than NR by a factor 4 for similar statistics

# PNR: Spin Asymmetry

- This magnetization-induced splitting between the Up-Up and Down-Down reflectivity's contains information regarding the magnetic depth profile of the thin film structure.
- Although not universally true, it is often the case that a larger splitting between the two cross sections indicates a larger magnetization of the film.
- Although we will always fit the reflectivity data itself, it is often helpful to plot the **spin asymmetry (SA)** of the reflectivity, defined as  $(U-D)/(U+D)$ , to better emphasize the magnetic features in the scattering, as shown below:

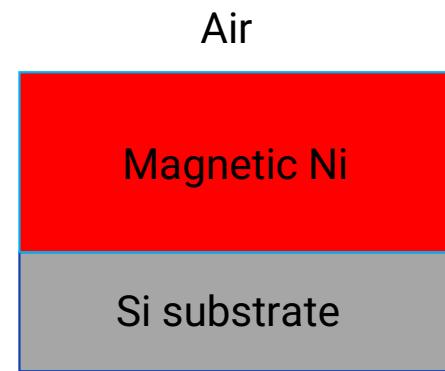
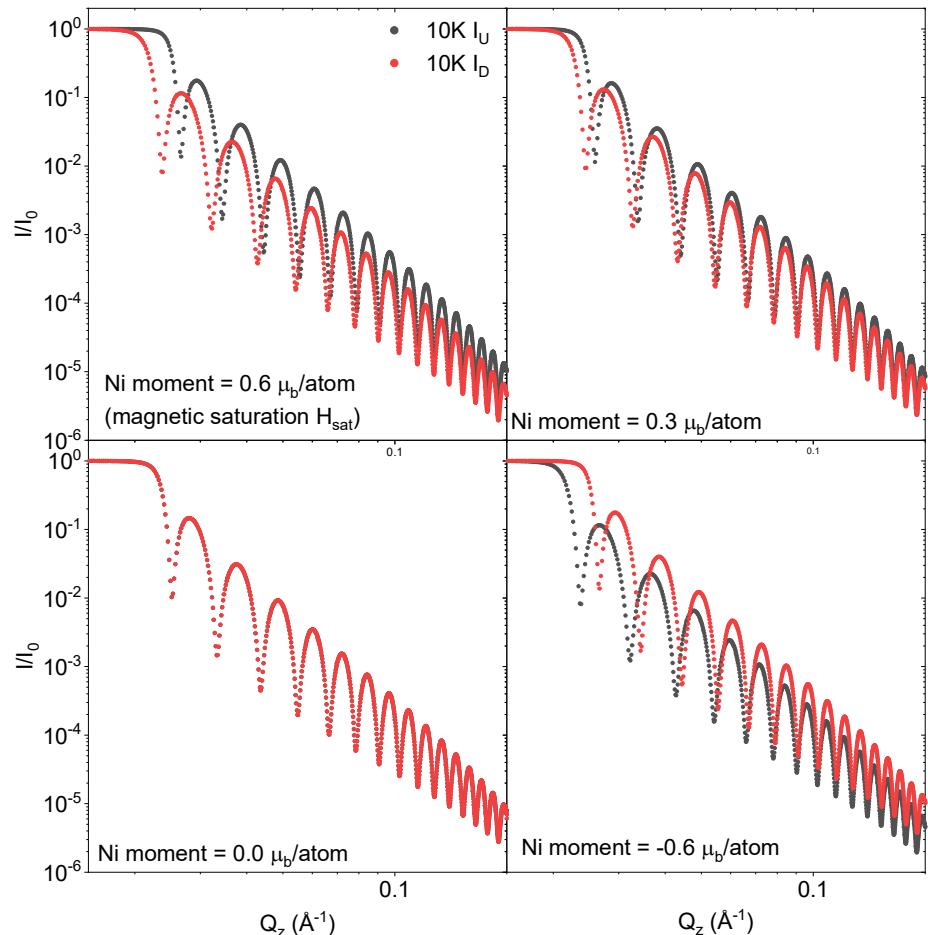


$$Spin\ Asymmetry = \frac{U - D}{U + D}$$



- This makes small magnetic changes a lot easier to see
- WARNING!!! Never fit the Spin Asymmetry exclusively on its own!!!!

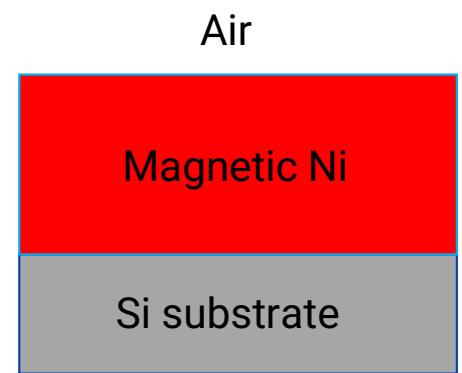
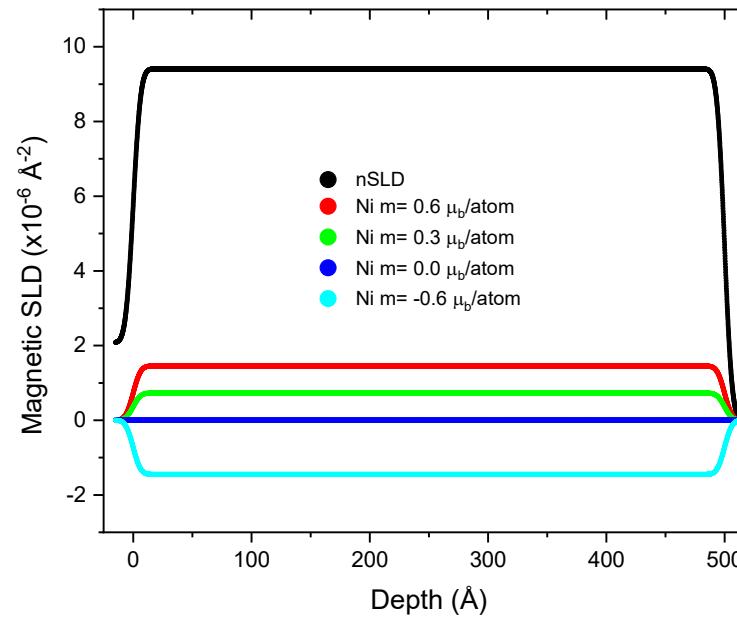
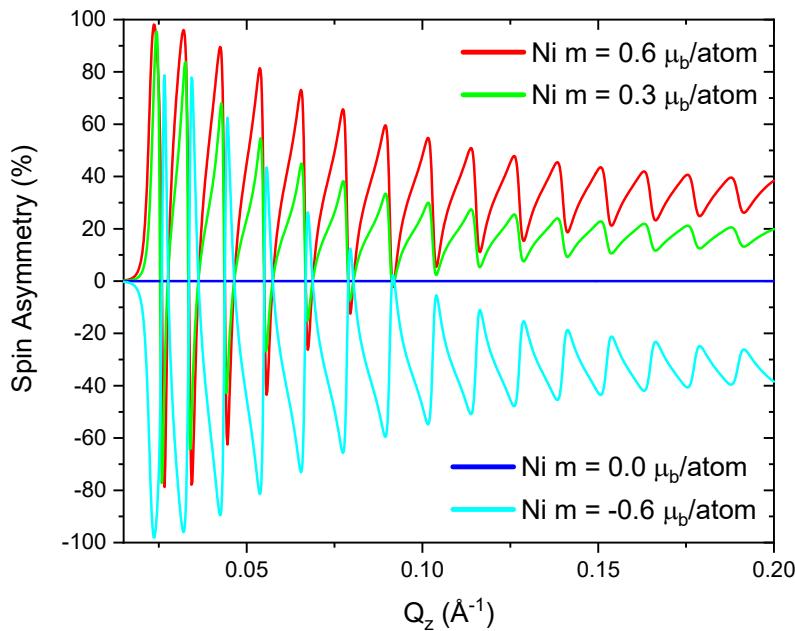
# PNR Magnetic SLD: Magnetic saturation to Negative Magnetic Saturation



- The Ni layer is 500 Å thick with the Silicon substrate and top Ni interface roughness's set to 5 Å rms ( $\sigma=5 \text{ \AA}$ ).
- The edges of the magnetism are commensurate with the Ni nuclear structure, i.e. matching the thickness and roughness exactly.

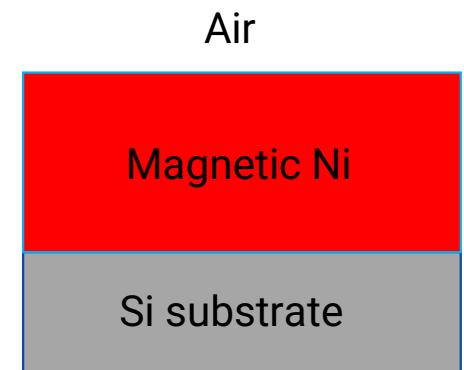
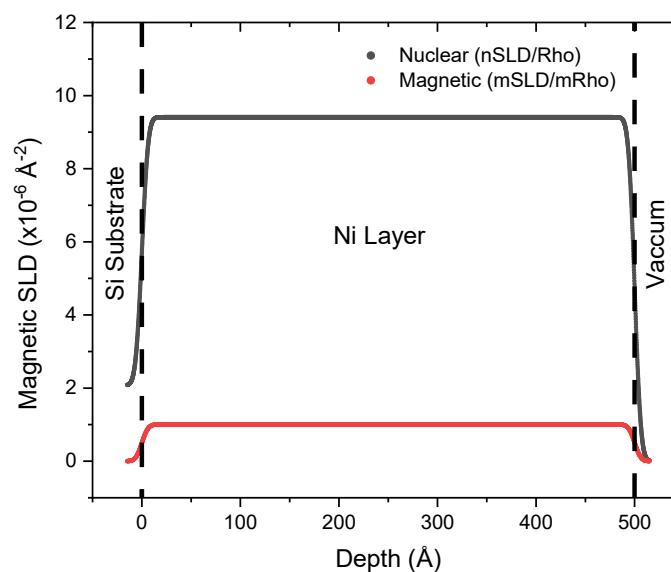
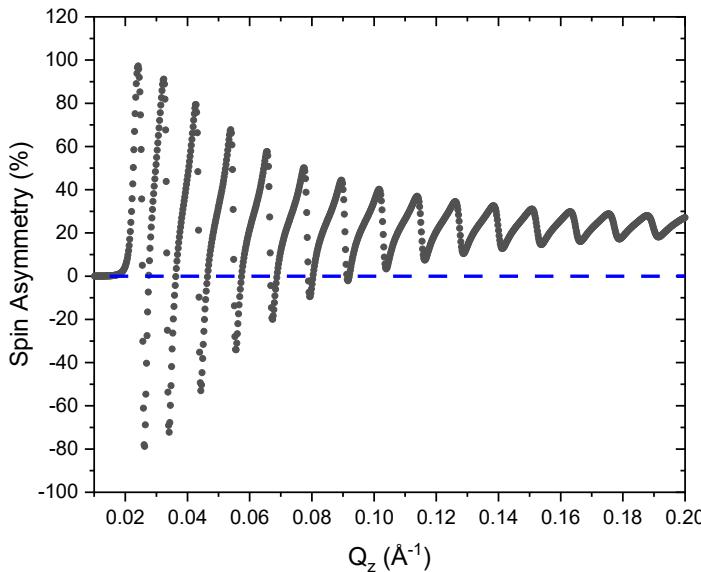
- Note the spin states have switched position for the negative magnetic moment  $-0.6 \mu_B/\text{atom}$

# PNR Magnetic SLD: Magnetic saturation to Negative Magnetic Saturation



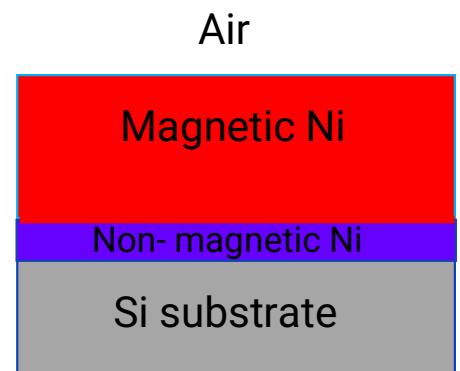
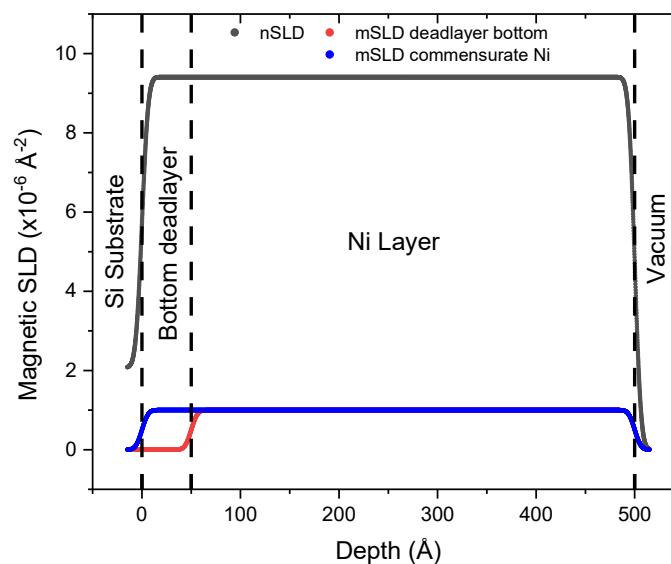
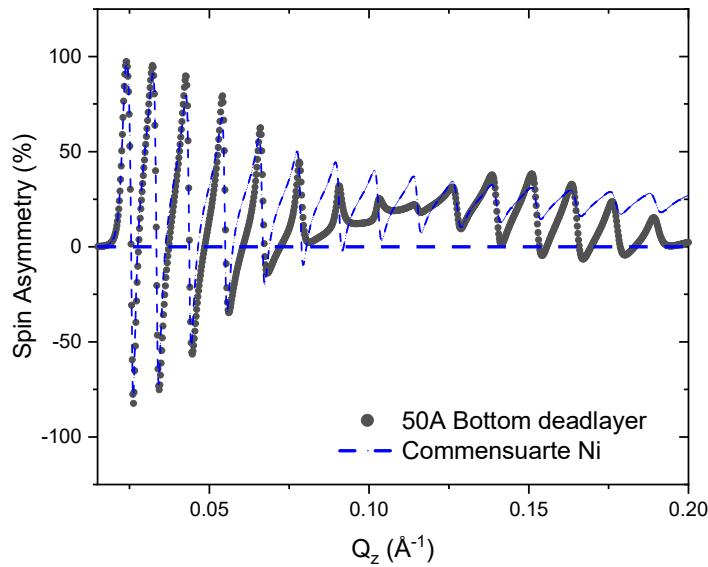
- The Ni layer is 500  $\text{\AA}$  thick with the silicon and top interface roughness set to 5  $\text{\AA}$  rms ( $\sigma=5 \text{\AA}$ ).
- It is much easier to see changes in the SA plot.
- The  $-0.6 \mu_b/\text{atom}$  SLD and SA are both flipped. This is the reverse saturated case the magnetisation of the sample is now antiparallel to the polarisation of the beamline.

# PNR :Magnetic Thickness: Commensurate Ni



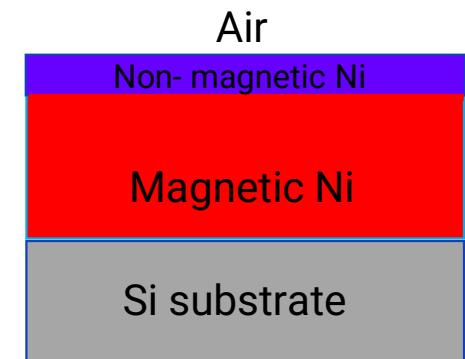
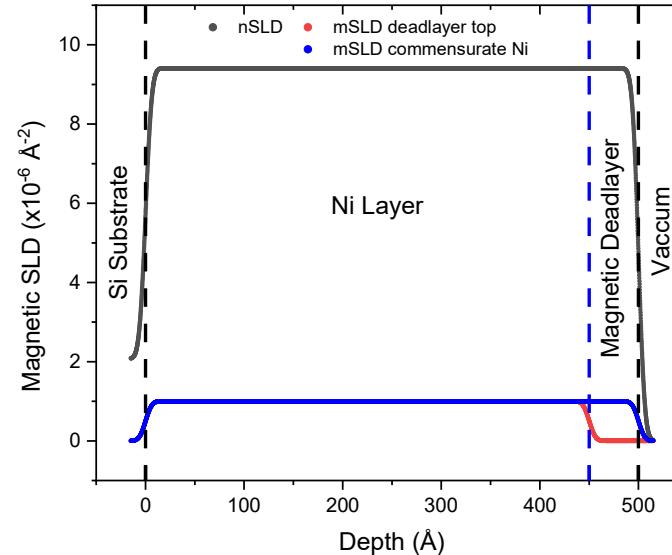
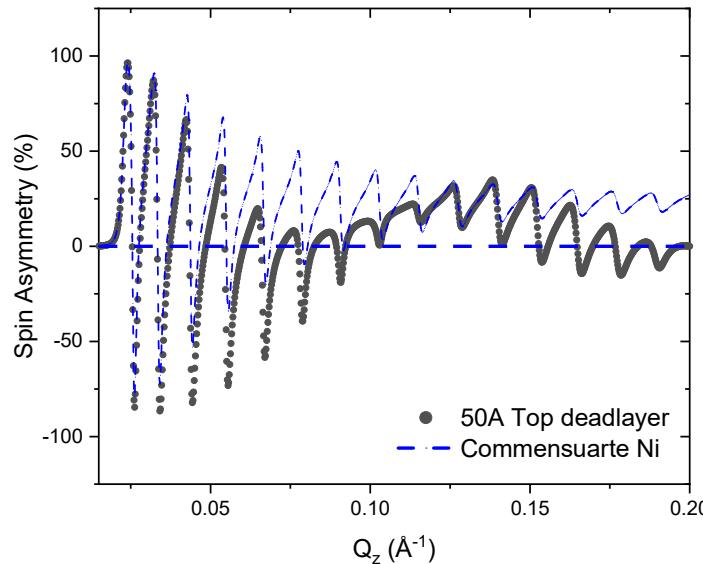
- The Ni layer is 500  $\text{\AA}$  thick with the silicon and top interface roughness set to 5  $\text{\AA}$  rms ( $\sigma=5 \text{\AA}$ ).
- The magnetism in the Ni is set to 0.6  $\mu_b/\text{atom}$ , the saturated case.
- The edges of the magnetism are commensurate with the Ni nuclear structure, matching the thickness.

# PNR Magnetic Thickness: Bottom magnetic dead-layer



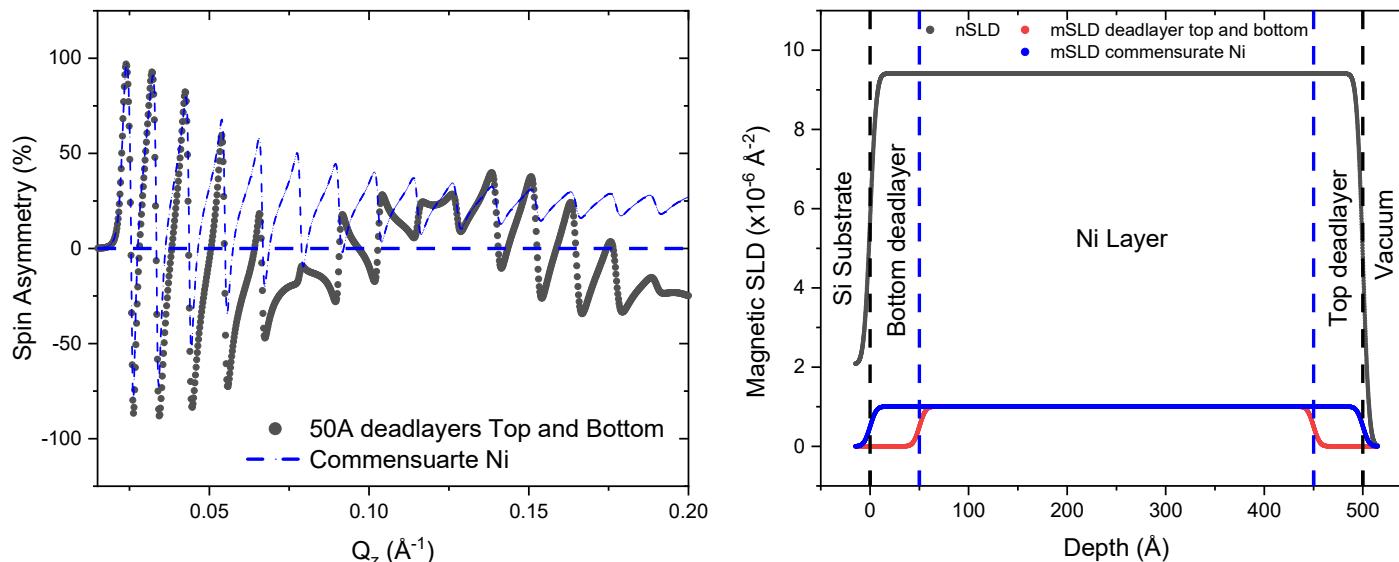
- The Ni layer is 500  $\text{\AA}$  thick with the silicon and top interface roughness set to 5  $\text{\AA}$  rms ( $\sigma=5 \text{\AA}$ ).
- 50  $\text{\AA}$  magnetic dead-layer at the bottom interface with the silicon substrate.
- The splitting in the PNR is modulated by a long range envelope function from the thinner dead-layer.

# PNR Magnetic Thickness: Top magnetic dead-layer

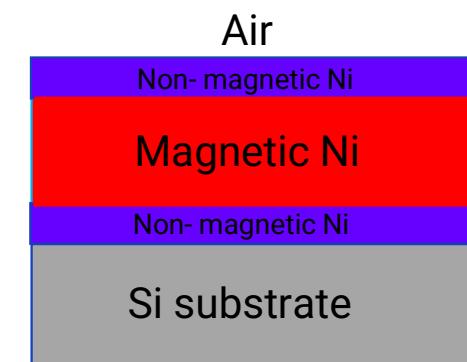


- The Ni layer is 500  $\text{\AA}$  thick with the silicon and top interface roughness set to 5  $\text{\AA}$  rms ( $\sigma=5 \text{\AA}$ ).
- 50  $\text{\AA}$  magnetic dead-layer at the top interface with the air.
- Easy to see using the SA that the envelope function shifts its modulation.

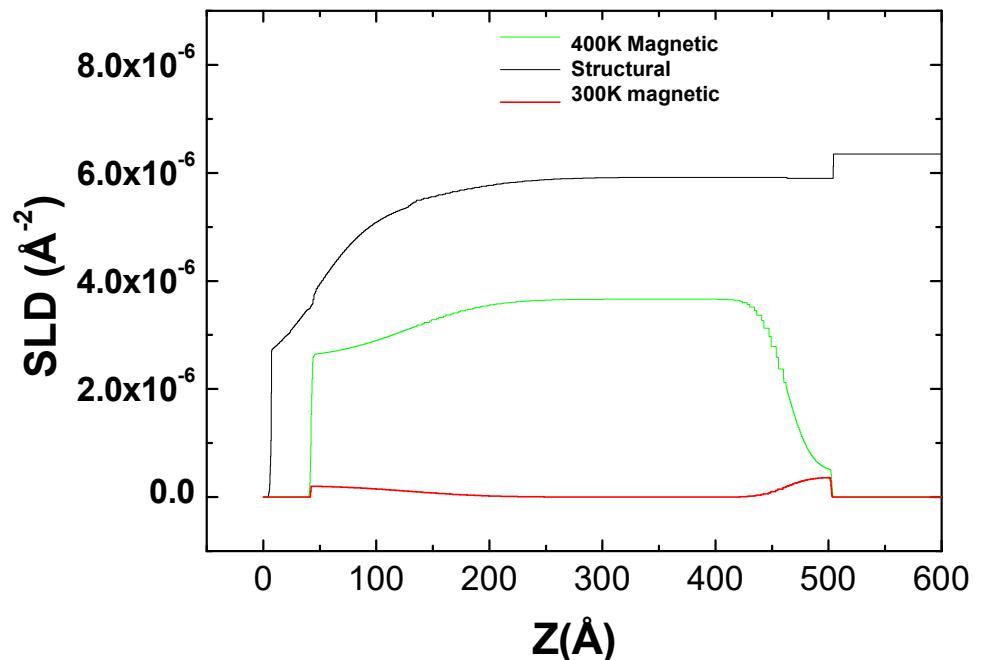
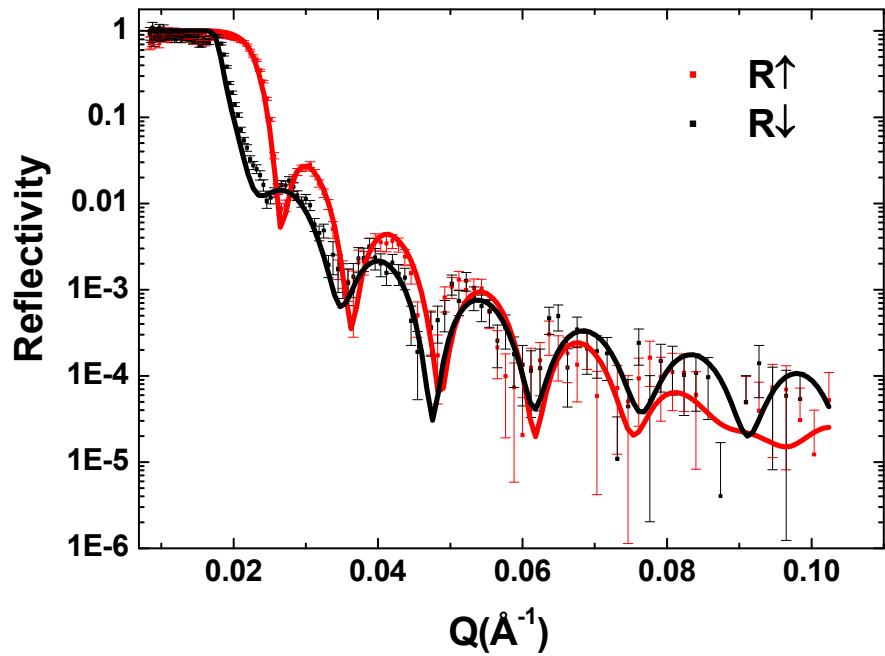
# PNR Magnetic Thickness: Top and bottom dead-layers



- The Ni layer is 500 Å thick with Silicon and top interface roughness of 5 Å ( $\sigma=5 \text{ \AA}$ ).
- 50 Å magnetic dead-layer at the top and bottom interfaces with the silicon substrate and air respectively.
- Easy to see using the SA that two envelope functions combine to change the modulation. Effectively now have three magnetic layers living in the same nuclear layer.
- NOTE: Dead-layers can be inverted, where the bulk becomes nonmagnetic, and the interfaces remain magnetic.



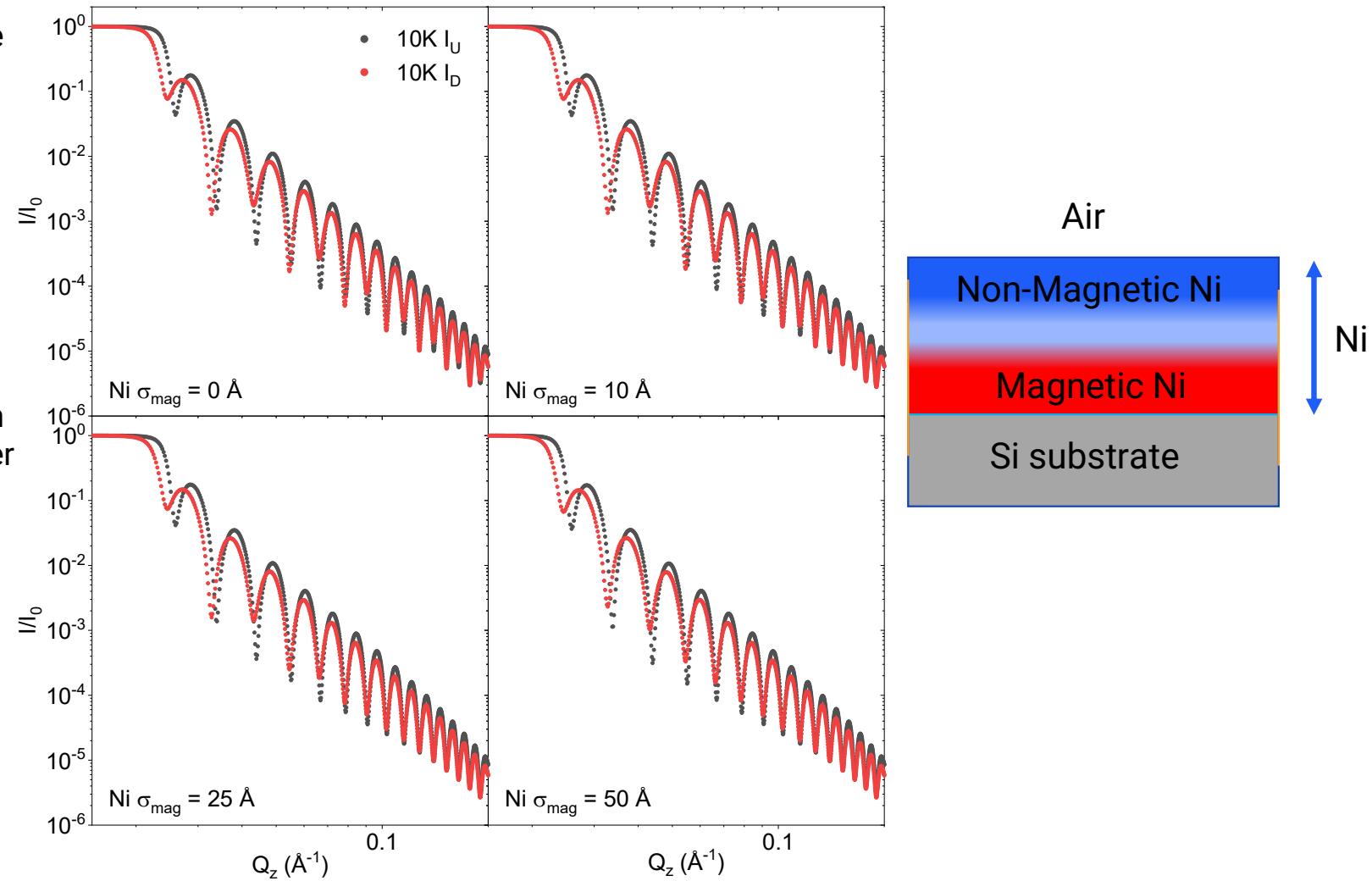
# PNR example: MgO(sub)/FeRh(50nm)/MgO(5nm)



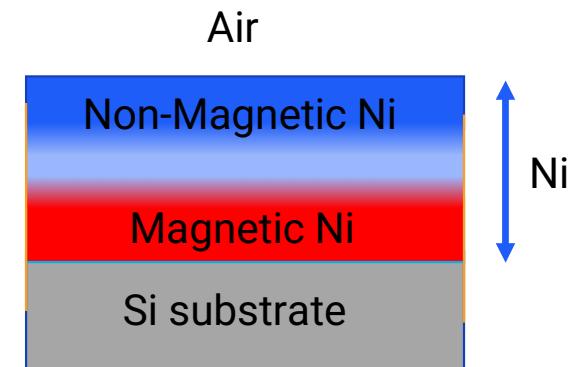
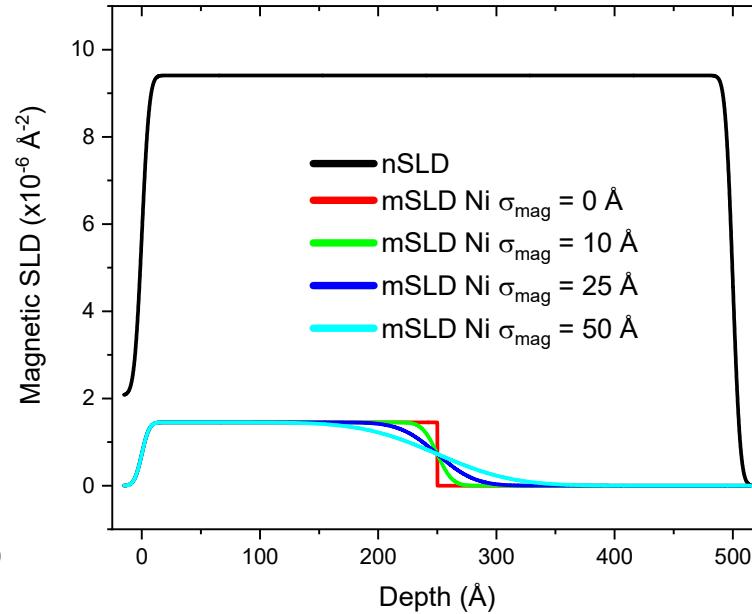
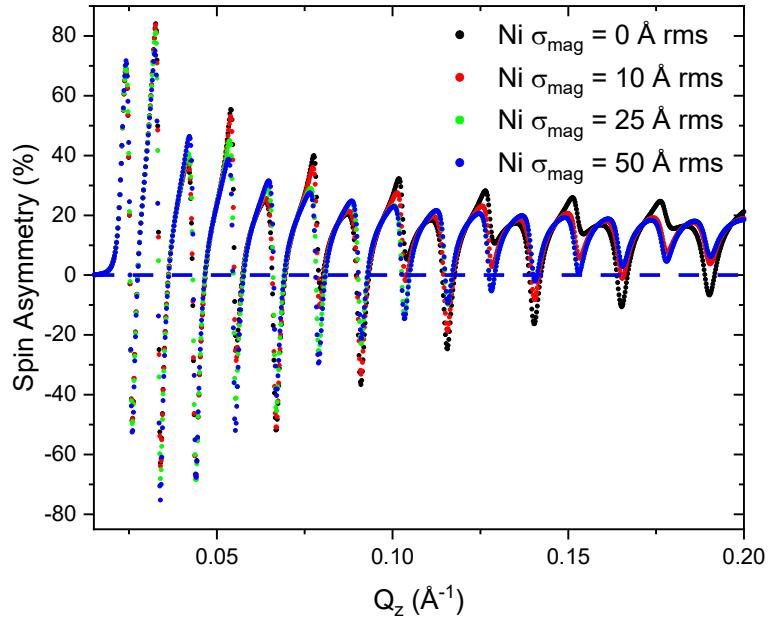
- FeRh has a AF/FM/P set of transitions with temperature. The  $T_c$  for the FM is 400K (100C).
- Magnetic SLD depth profile, shows how influence of substrate and surface effect magnetism in AF phase. FM persists at in the interface regions to low temperatures.

# PNR Magnetic roughness:

- Magnetic roughness treated the same as structural roughness. Applied to the mSLD only.
- Modelled as a gaussian interface.
- Not the only functional form for a magnetic interface.
- Effects are much more subtle in the reflectivity curves and harder to spot.



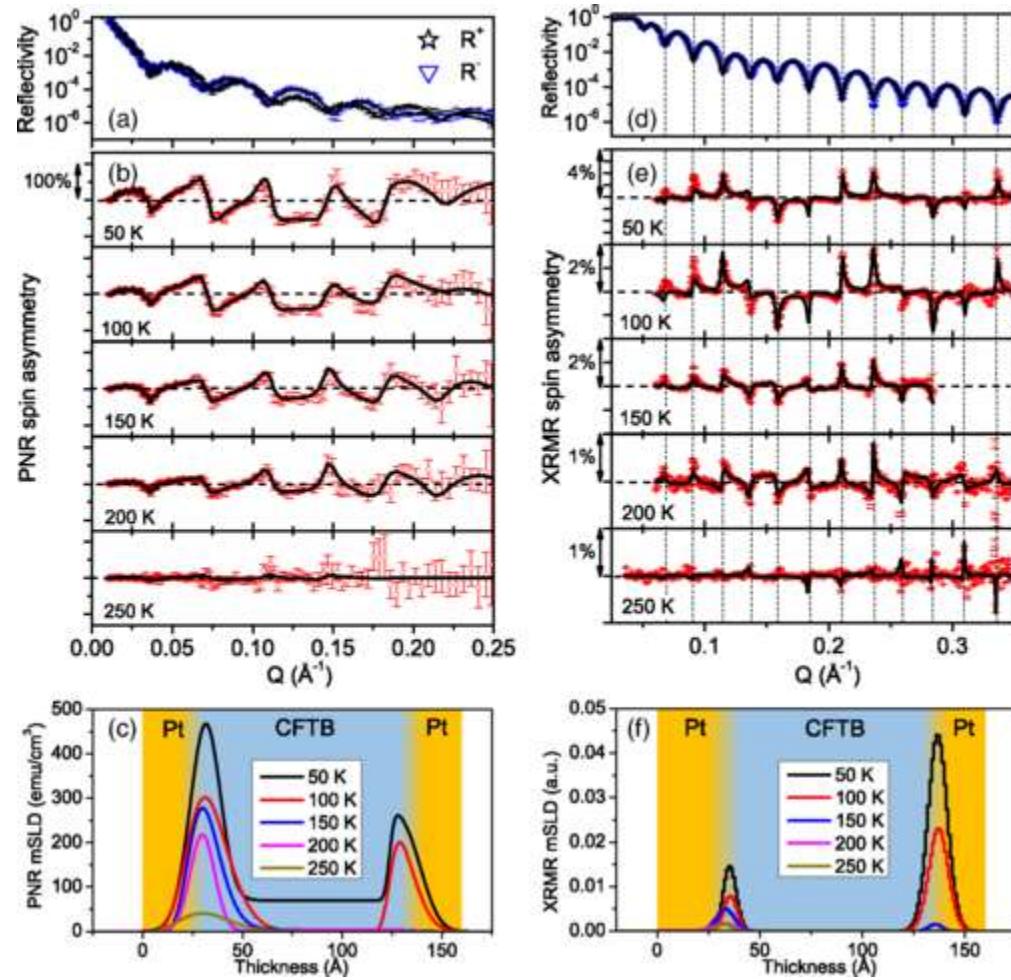
# PNR Magnetic roughness:



- The Ni layer is 500  $\text{\AA}$  thick with the silicon and top interface roughness set to 5  $\text{\AA}$  rms ( $\sigma=5 \text{ \AA}$ ).
- 250  $\text{\AA}$  magnetic dead-layer starting in the middle of the layer which is magnetically roughened via a Gaussian profile.
- Effects are more subtle but easily seen at High Q in the SA

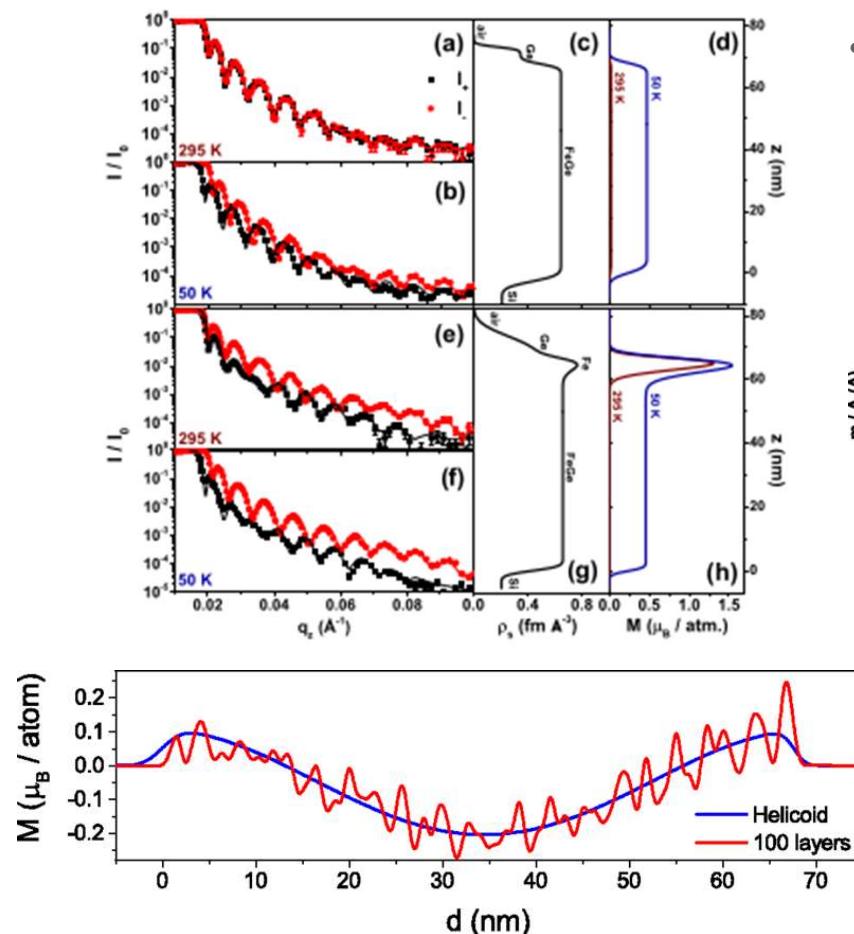
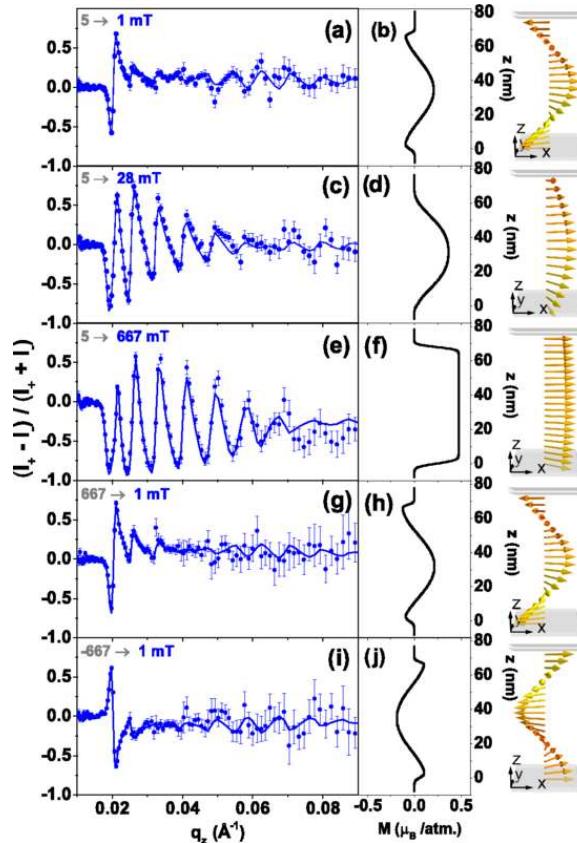
# PNR examples CFTB/Pt proximity effects

- CoFeTaB – amorphous FM, low magnetisation and tuneable  $T_c$  with tantalum concentration
- Polarised neutron reflectivity (PNR) using Polref instrument @ ISIS, data fitted using GenX
- Scattering sensitive to structure and magnetism
- Magnetic signal here only from CoFeTaB layer: moment on Pt is below sensitivity limit.
- Authors use XRMS scattering to probe the Pt. This is a good example of the complementary use of different scattering techniques.
- The effects are a combination of density changes and magnetic roughness.

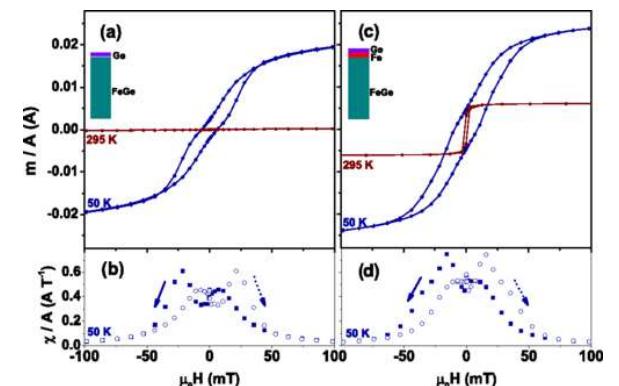


O. Inyang et. al. Phys. Rev. B 100, 174418

# PNR Examples: Spin Helix in FeGe thin films and FeGe/Fe multilayers (DMI)

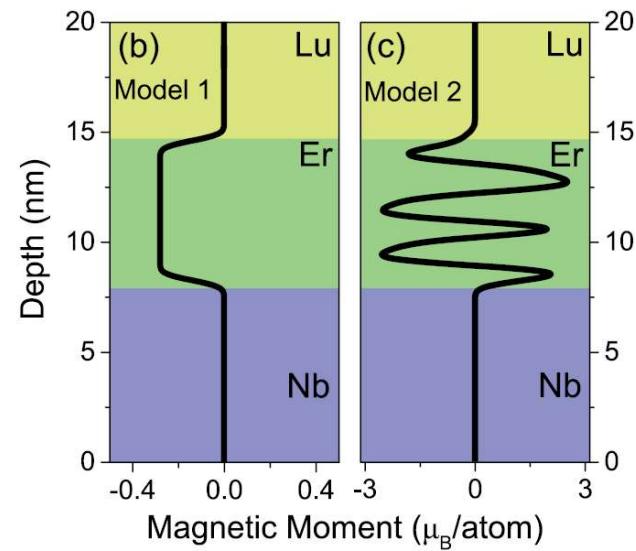
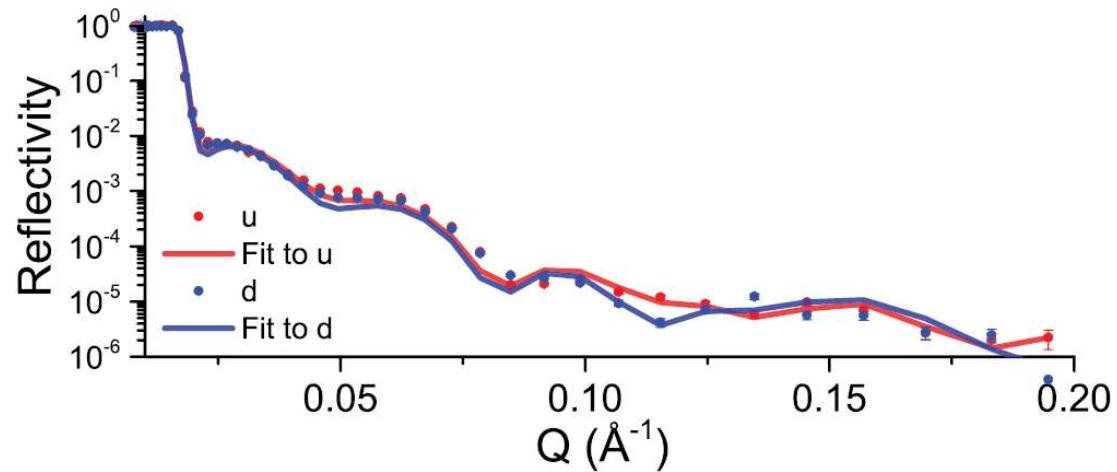


- Example of the combination of PNR with Transport/Magentometry and XRD/XRR



- N.A. Porter et al PRB 92, 144402 (2015)
- C. S. Spenser et al PRB 97, 214406, (2018)

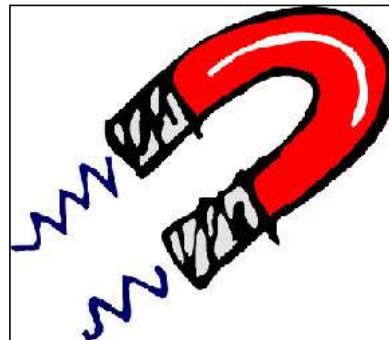
# PNR example: Er Spin Spiral



- Er based Spin spiral in a think magnetic layer.
- Good example of the use of a Null hypothesis to indicate the presence of a magnetic structure.

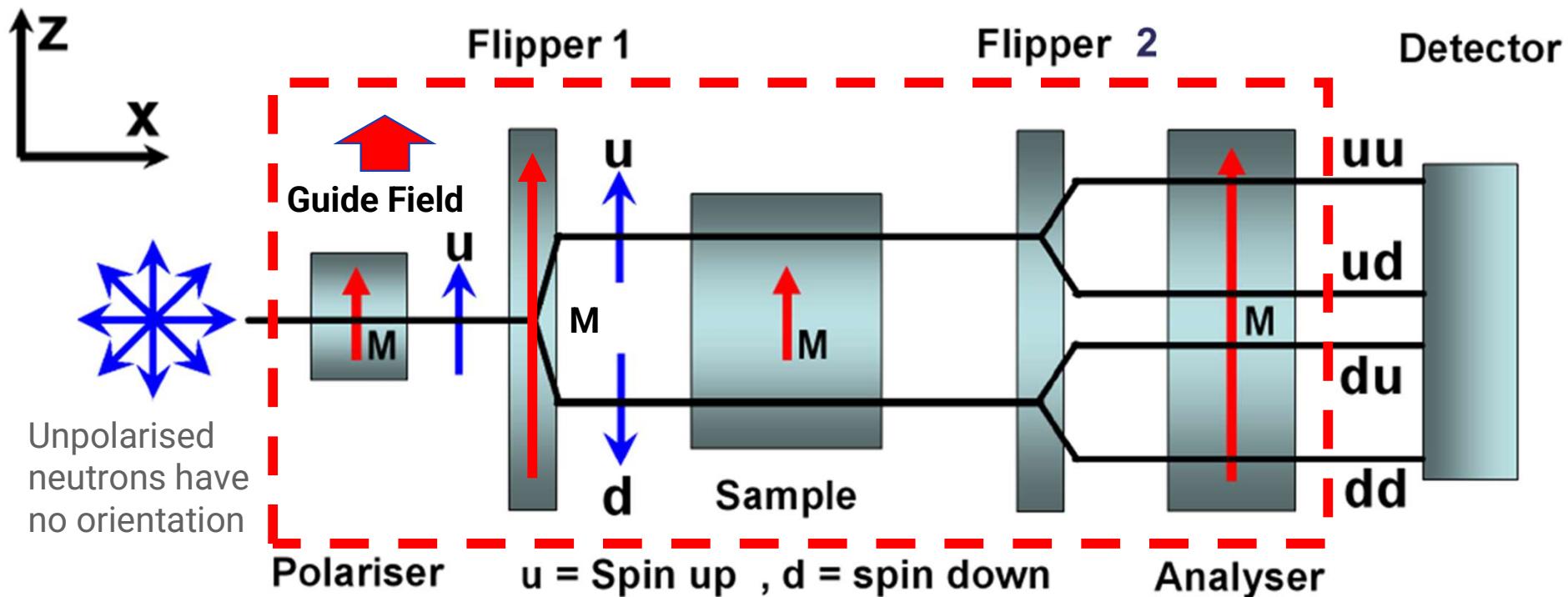
# Polarisation analysis (PA)

- NR measures the **Nuclear** scattering length density profile.
- PNR measures the **Magnetic** scattering length density profile.



- PA measures the **Magnetic** scattering length density profile and **Magnetic vector** in the  $xy$  plane of the sample as a function of depth!

# Polarisation analysis (PA):



- Second flipper and Analyser added to the system. **Experiments now takes a factor 8 minimum longer!**
- Now measure 4 spin states with 50% of the initial flux! PA experiments very tough!
  - UU and DD – Non Spin flip channels
  - UD and DU – Spin flip channels

# Polarisation analysis (PA):

- Only magnetic scattering can cause spin flip scattering.

$$\left. \begin{array}{l} \mathbf{U}^{uu} = N + M_{\perp,z}, \\ \mathbf{U}^{dd} = N - M_{\perp,z}, \\ \\ \mathbf{U}^{ud} = M_{\perp,x} + iM_{\perp,y}, \\ \mathbf{U}^{du} = M_{\perp,x} - iM_{\perp,y}, \end{array} \right\} \begin{array}{l} \text{Non Spin Flip} \\ \text{scattering (NSF)} \\ \\ \text{Spin Flip} \\ \text{scattering (SF)} \end{array}$$

- By measuring the 4 spins states uu, dd, ud and du, the in-plane orientation of the magnetism  $\mathbf{M}$  is obtainable.
- The ratio of Non Spin Flip (NSF) to Spin Flip (SF) scattering scales with the angle of  $\mathbf{M}$  in the plane of the sample.

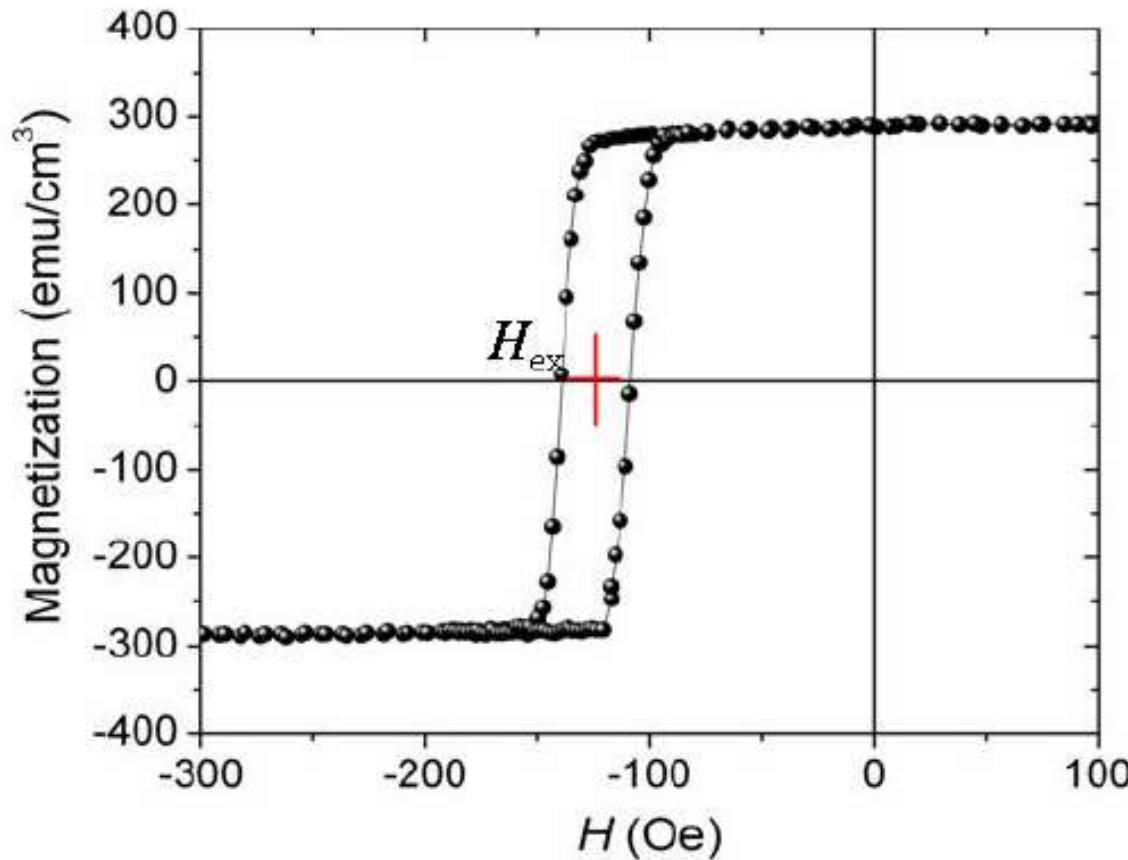
$$b = b + p \sin \phi$$

$$p_m \cos \phi = p_x$$

- Bland et al, Phys Rev B, 46, 3391 (1992)
- Zabel et al Physica B 276-278, 17 (2000)
- R. M. Moon et al Phys Rev, 1969, 181, 920-931
- S. Blundell et al, JMMM, 1993, 121, 185-188
- Bland et al, Phys Rev B, 46, 3391 (1992)

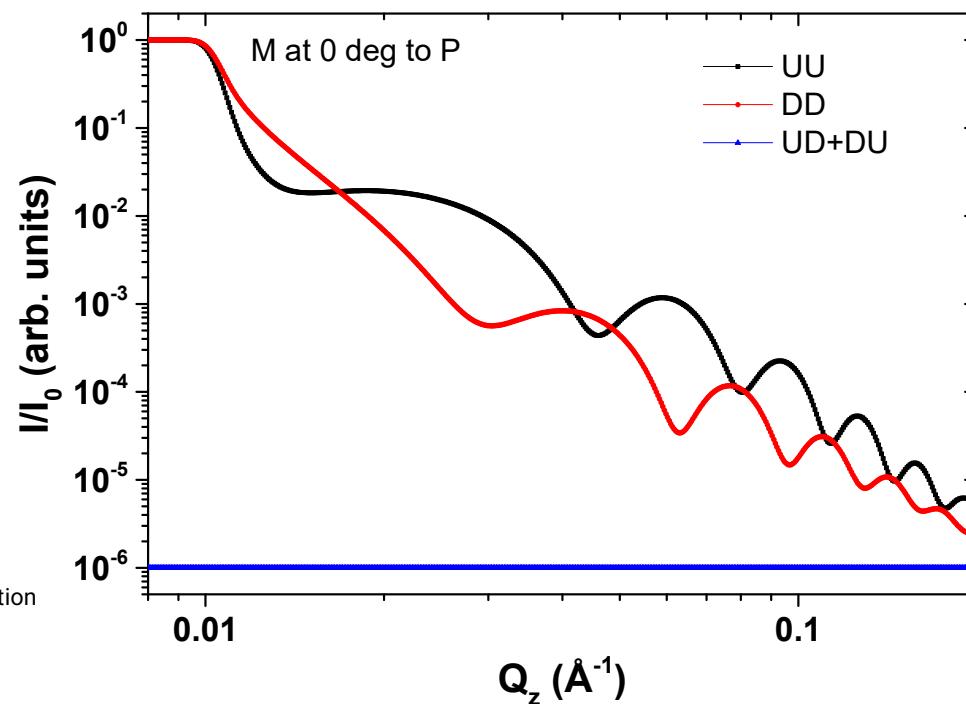
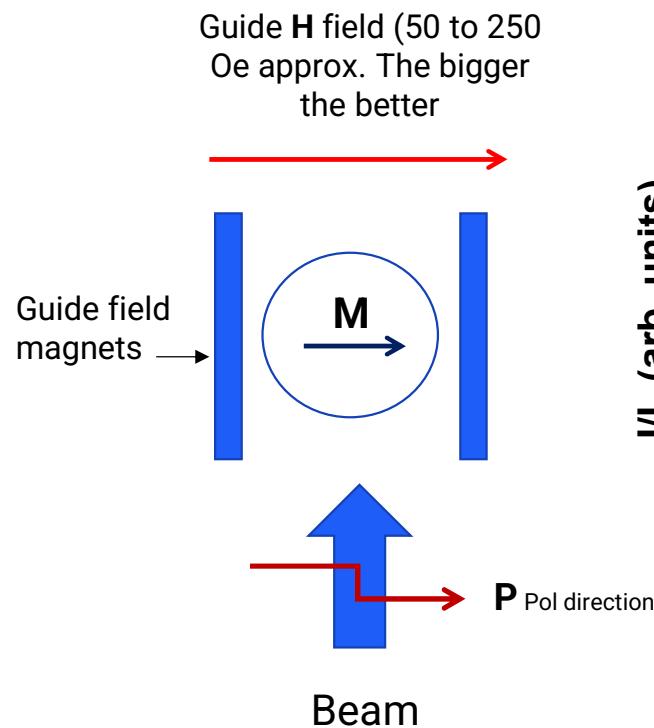
- G. L. Squires introduction to the Theory of Thermal neutron scattering
- Modern Techniques for Characterizing Magnetic Materials Edited by Yimei Zhu, Springer
- Neutron Scattering form Magnetic Materials, editor Tapan Chatterji, Elsevier

# Polarisation Analysis (PA): Test system



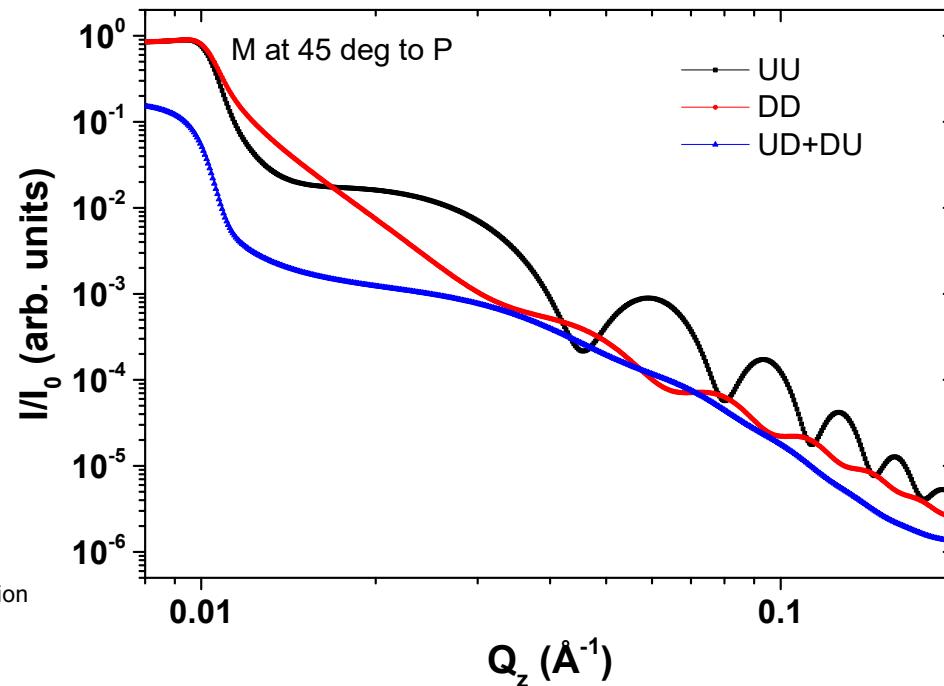
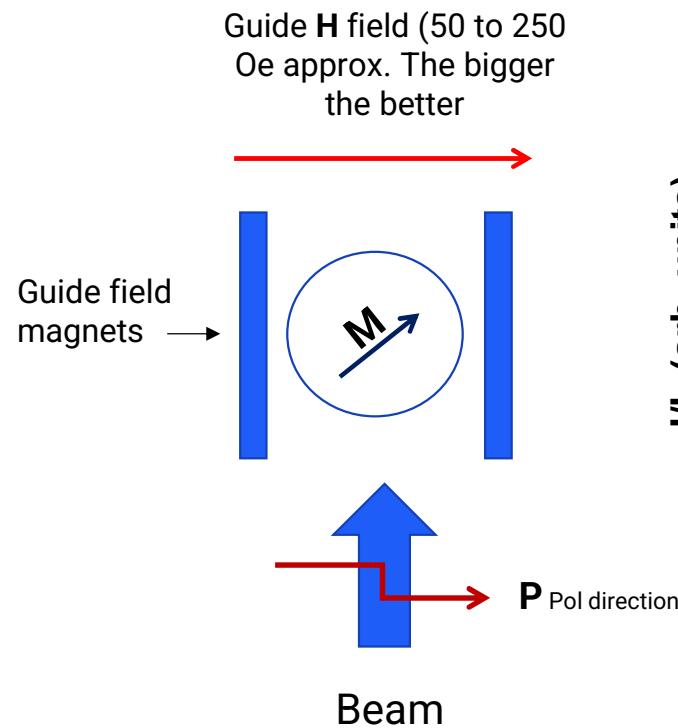
- Test Case: proto exchange bias (EB) sample
- EB happens when an antiferromagnet is put next to a FM.
- The effect is to pin the FM in one direction.
- If a small guide field approx. 10 Oe (0.001T) is used then the sample can be rotated without  $\mathbf{M}$  rotating to follow the guide field.
- Normally sputtered Co is very soft and amorphous/polycrystalline so has very low anisotropy, so no preferred direction and will rotate to follow any applied magnetic field.
- Placed next to an  $\text{IrMn}_3$  antiferromagnet it will be pinned in one direction.

# Polarisation Analysis Example 1: 0 Deg rotated M



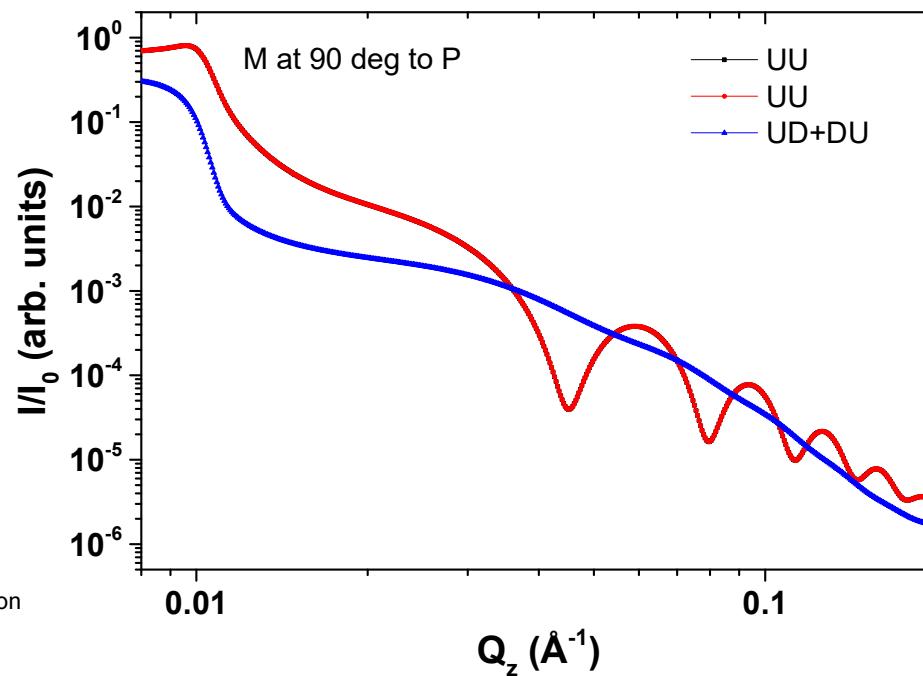
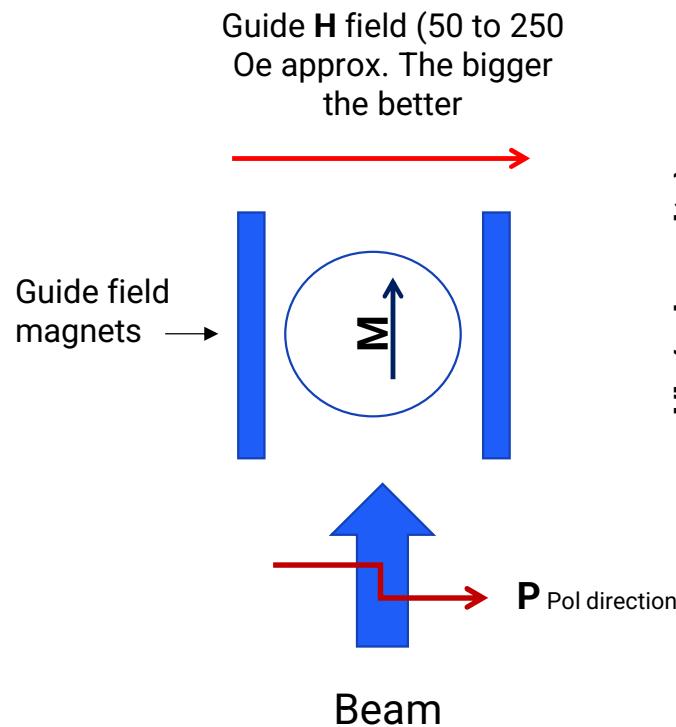
- Non spin flip case, only UU, DD states will can scatter.
- Zero spin flip

# Polarisation Analysis Example 2: 45 Deg rotated M



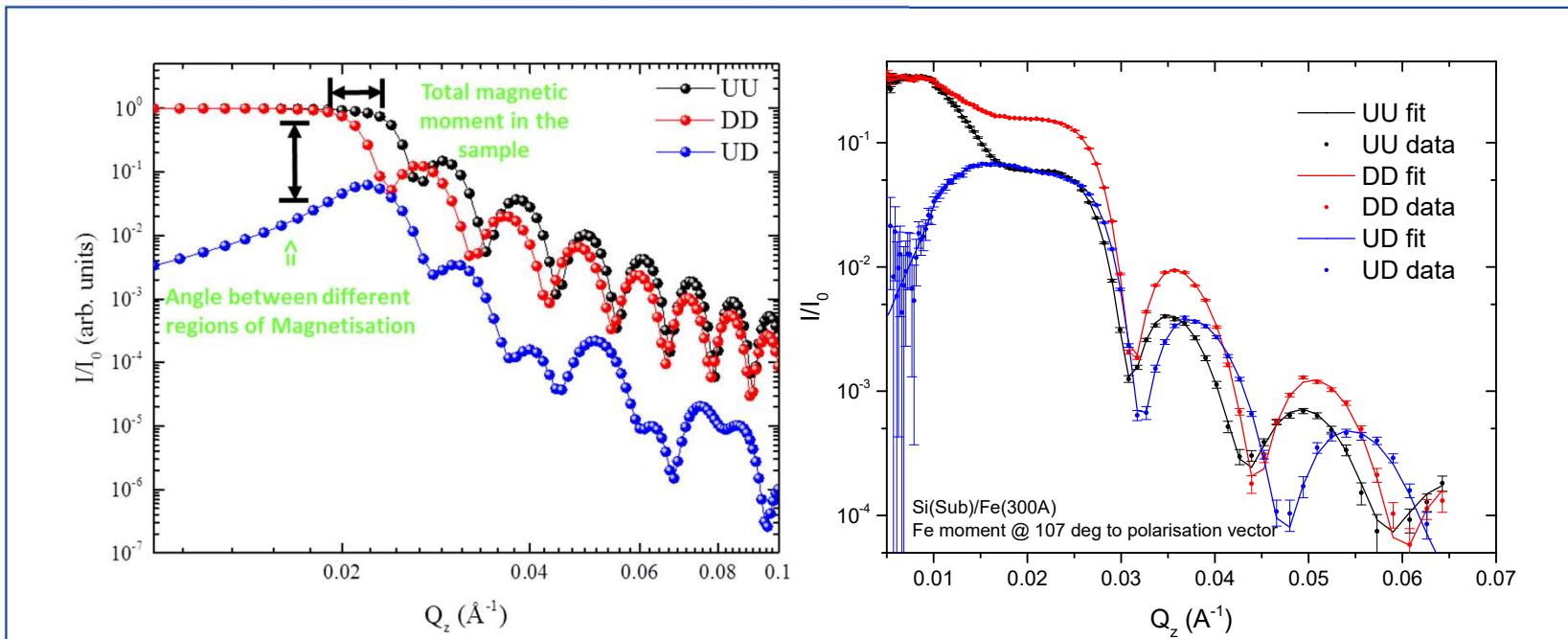
- Non spin flip UU, DD splitting reduced.
- Spin flip UD, DU is increased. In the specular case they should be the same.

# Polarisation Analysis Example 3: 90 Deg rotated M



- Non spin flip scattering now purely non-magnetic and UU and DD show no spin splitting nuclear scattering only.
- Spin flip UD, DU scatter is maximised

# Polarisation Analysis (PA): Summary



- Polarisation analysis tells you the angle of the Magnetisation in the plane of your sample as a function of depth. It's a depth dependent in-plane vector magnetometer!
- It also provides the nuclear (structural) and magnetic density depth profile.
- But it takes longer than PNR taking a factor 8 minimum longer than NR for equivalent statistics.
- Warning PA experiments are tough going! You really need to have to do the measurement and really need to know at what fields and temperatures to measure at!

## Some SANS examples Courtesy of Nina Steinke of D33 at the ILL

- I am not a big expert in Magnetic SANS or PolSANS for these I direct detailed questions to Nina!
- Magnetic SANS is not the same as PolSANS!
- In Magnetic SANS the neutron beam is not polarised, but the neutrons can still scatter magnetically!
- PolSANS allows you to measure direction and size of the magnetic moments like reflectivity but it's harder to do. It's not the same as PNR/PA.
- Here are some Nina Examples



[www.isis.stfc.ac.uk](http://www.isis.stfc.ac.uk)

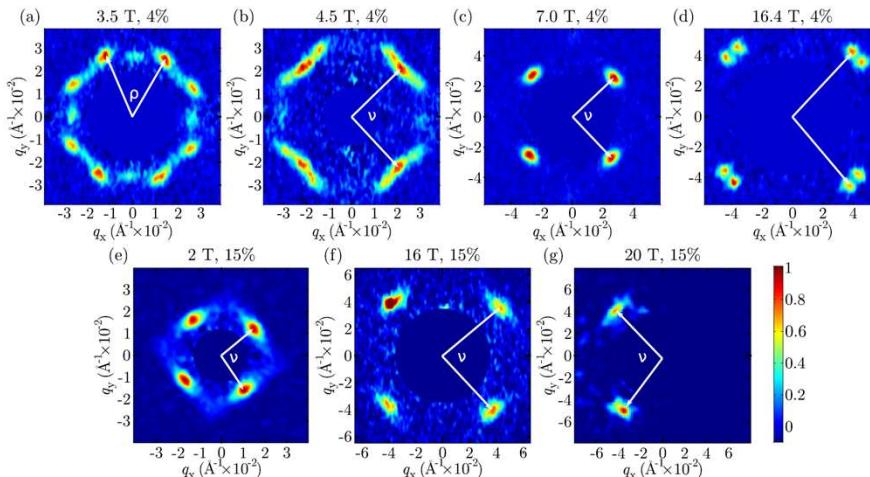


[@isisneutronmuon](#)



[uk.linkedin.com/showcase/isis-neutron-and-muon-source](https://uk.linkedin.com/showcase/isis-neutron-and-muon-source)

# Characterising high TC superconductivity in Ca-doped YBCO through vortex lattice diffraction.



d-wave nature of superconducting gap is unaffected by Ca doping, no s-wave signature. Field transitions are shifted to lower fields, due to weakening of 1-D superconductivity Cu-O chains in doped compounds.

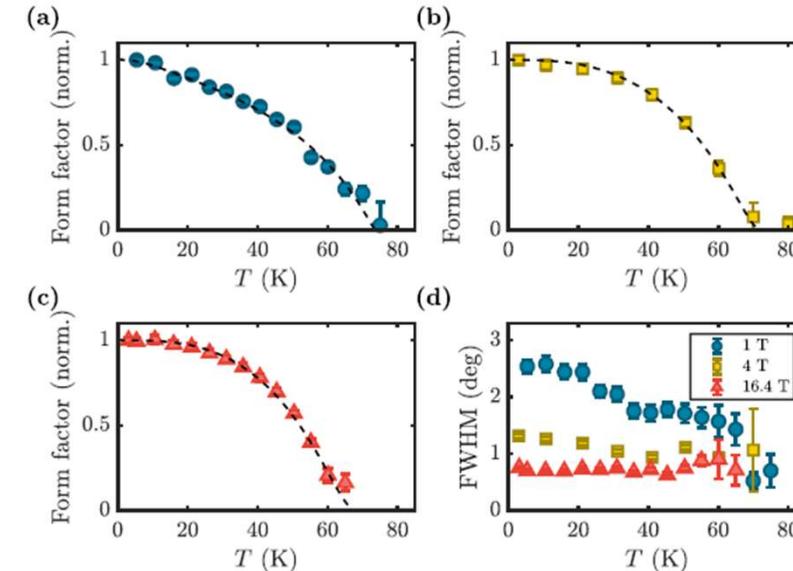


FIG. 6. Vortex lattice form factor as a function of temperature in an applied field of (a) 1 T, (b) 4 T, and (c) 16.4 T. The solid line in (a) is a fit to the anisotropic London model using a *d*-wave gap described in the text. (d) Variation of the rocking curve FWHM as a function of temperature for the data presented in (a)–(c).

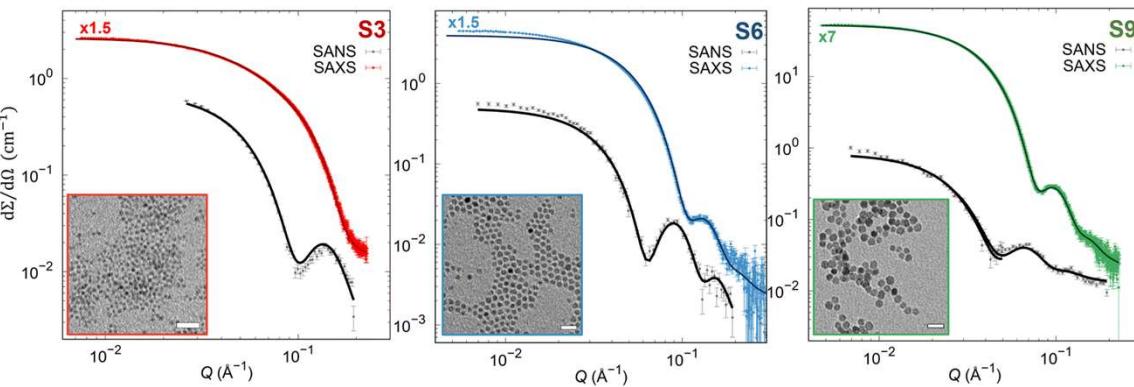
Studying the VL gives detailed information on the superconducting state: gap symmetry, order parameter etc.



Cite this: *Nanoscale Adv.*, 2023, 5, 4563

## Size dependence of the surface spin disorder and surface anisotropy constant in ferrite nanoparticles<sup>†</sup>

Marianna Gerina,<sup>ID a</sup> Marco Sanna Angotzi,<sup>ID b</sup> Valentina Mameli,<sup>ID b</sup> Veronika Gajdošová,<sup>c</sup> Daniel N. Rainer,<sup>ID d</sup> Milan Dopita,<sup>e</sup> Nina-Juliane Steinke,<sup>f</sup> David Aurélio,<sup>e</sup> Jana Vejpravová<sup>ID e</sup> and Dominika Zákutná<sup>ID \*a</sup>



Magnetic nanoparticles for technologies such as:

- Magnetic recording
- Lab on a chip applications
- Magnetic resonance imaging
- Fluid magnetic hyperthermia (cancer) treatments

As magnet size approaches nanoscale, disorder effects become increasingly important.

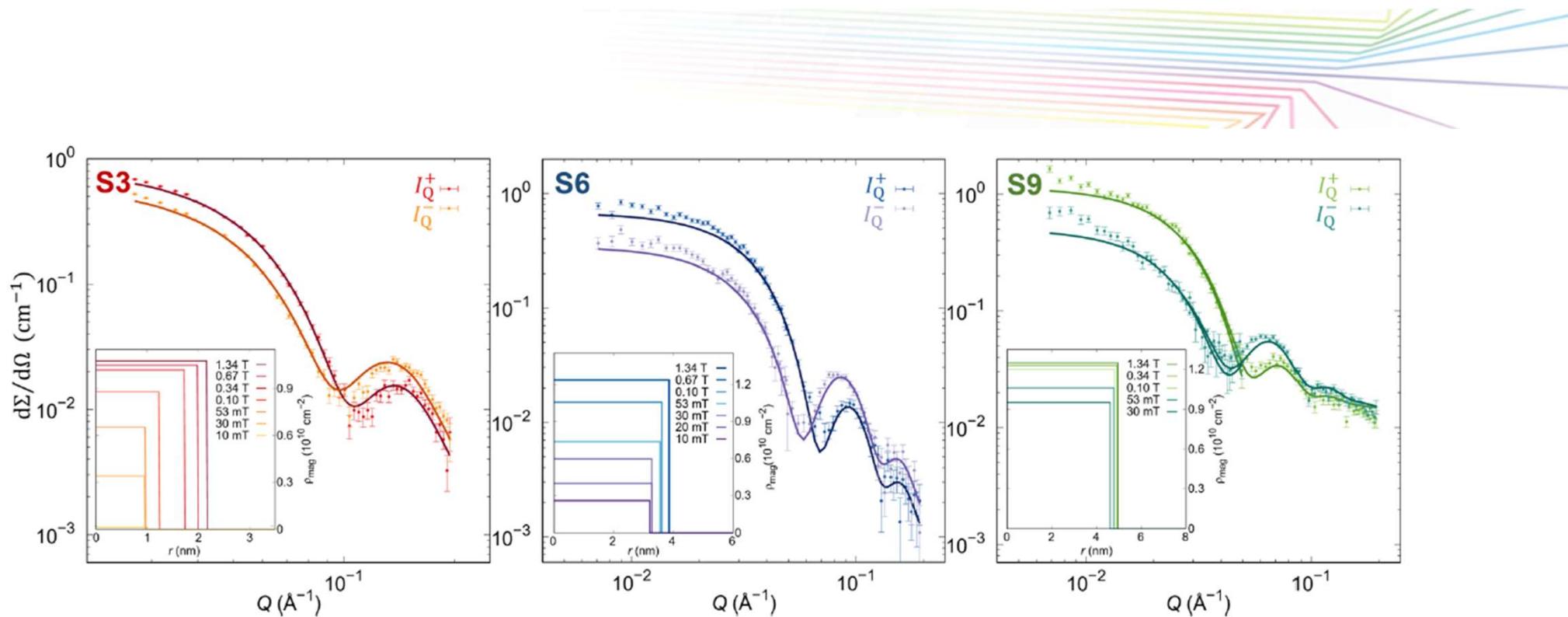


Fig. 2 SANSPOL scattering cross sections (points) for the polarization  $I_Q^-$  and  $I_Q^+$  with core–shell–dead layer form factor refinements (full lines) at 1.34 T. (Insets) Obtained radial distribution of  $\rho_{\text{mag}}$  at different applied magnetic fields.

Use polarised SANS to extract magnetisation distribution inside the particle, surface disorder and surface anisotropy constant.

# Magnetic Scattering Rule:

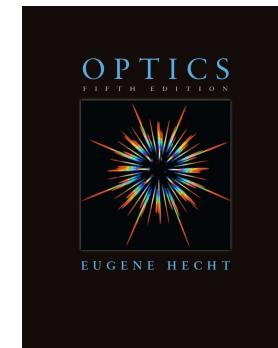
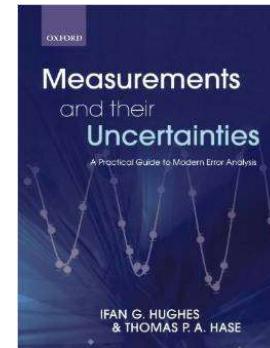
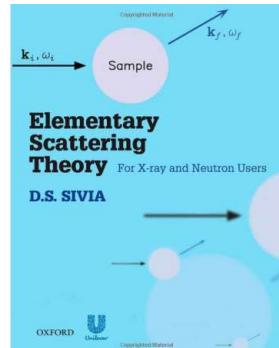
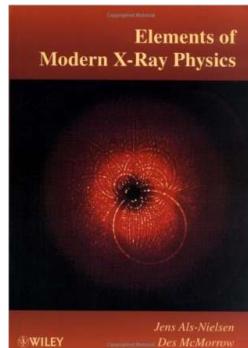
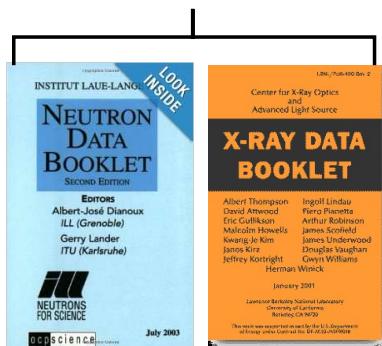
- The non-spin-flip scattering is sensitive only to those components of the magnetisation parallel to the neutron spin
- The spin-flip scattering is sensitive only to those components of the magnetisation perpendicular to the neutron spin.
- The ratio of non spin-flip to spin-flip scattering give the angle in the plane of the sample.

NB This is one of those points that you should take away with you. It is the basis of all magnetic polarization analysis techniques.

Courtesy of Ross Stewart, ISIS

# Useful books: These are actually helpful when doing experiments!

Free on web



<http://xdb.lbl.gov/>

Excellent for x-ray magnetic scattering.

Deals with all theory that's needed for doing scattering experiments.

Deals with all stats needed for dealing with SANS/NR data.

Deals with a lot of basic optics theory.

These are the books I learned from but there are many out there.

Thank you for listening



[www.isis.stfc.ac.uk](http://www.isis.stfc.ac.uk)



[@isisneutronmuon](https://twitter.com/isisneutronmuon)



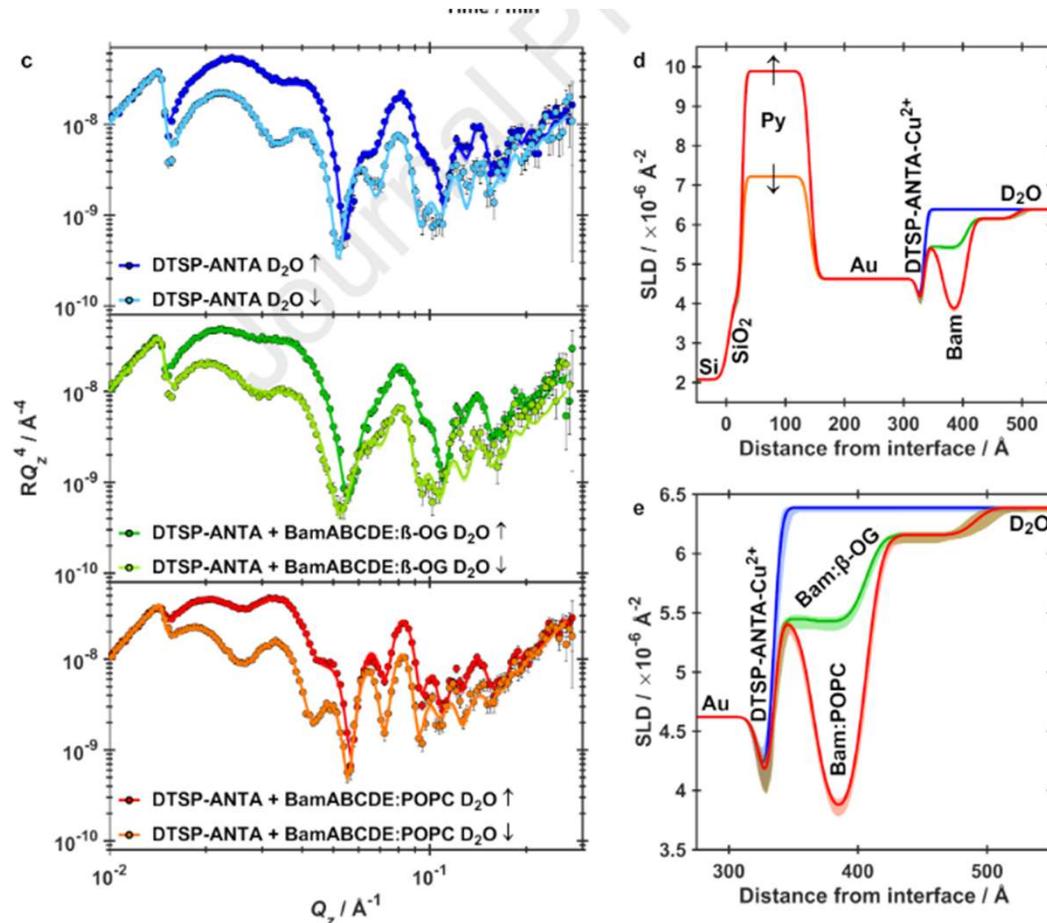
[uk.linkedin.com/showcase/isis-neutron-and-muon-source](https://uk.linkedin.com/showcase/isis-neutron-and-muon-source)

# PNR/PA Practical points for experiments: Soft matter Magnetic contrast.

- Reflectivity is basically a battle for contrast!
- In NR for Chemistry and Biology isotopic contrast is a real boon. Can mix H<sub>2</sub>O and D<sub>2</sub>O to contrast to match out layers and beat the inverse phase problem. Makes fitting a lot easier!
- Deuteration not possible for some systems. To expensive or too difficult.
- Magnetic contrast can then be used. Magnetic reference layer is used like Py or Fe. This gives two contrast via that magnetic layer.
- The technique can be used with isotopic contrast as well to reduce the ambiguity of analysis further.
- Warning PNR takes longer to measure (x4) it might be worth measuring more isotopic contrasts rather than one magnetic contrast.

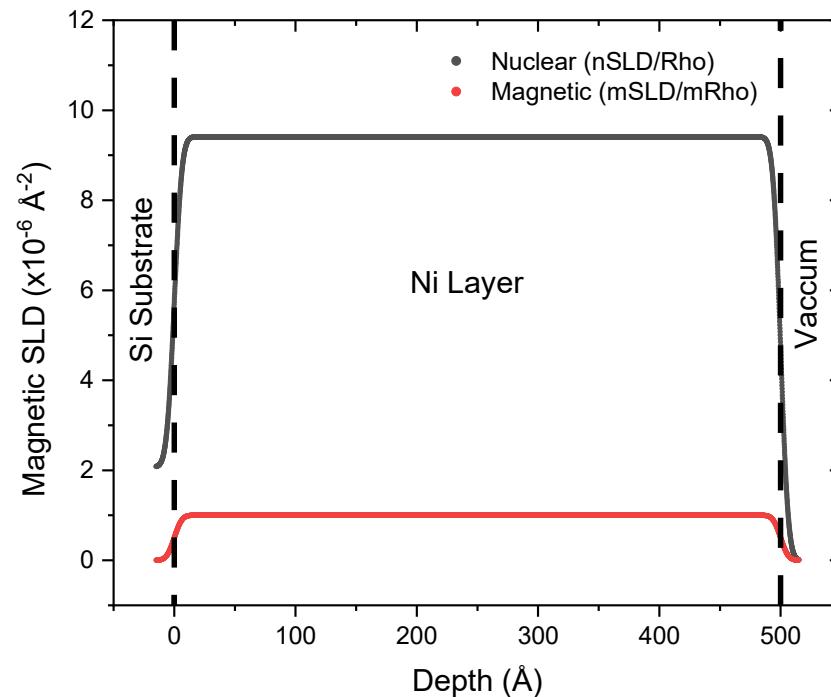
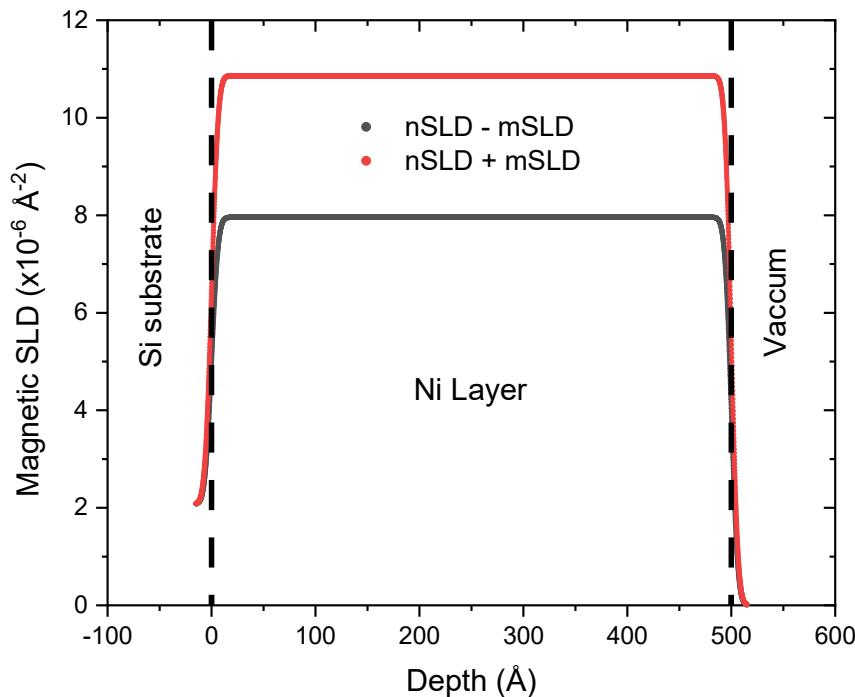
Why reference layers and  
isotopic/magnetic contrast variation  
works:

- A. Koutsioubas, J. Appl. Cryst. (2019). 52, 538–547
- C.F. Majkrzak *et. al.*, Langmuir 2003, 19, 7796-7810



# PNR/PA Practical points for experiments:

- Plotting PNR SLD profiles for Hard Condensed Matter (HCM) and Soft Matter (SM) experiments is different as they have different aims.



- In SM the mSLD is added to the nSLD as the magnetic profile is effectively irrelevant its just there to add another contrast. This is what the spin up and down neutrons actually interact with in reality.
- In HCM the magnetic mSLD profile is the thing that is actually wanted so it is best to deconvolve the two into separate mSLD and nSLD curves.

# PNR/PA Practical points for experiments:

Experimental planning: Count times and picking measurements!

- Technique:

- NR is quick
- PNR is x4 time slower than NR
- PA is x8 -x16 times slower than NR (is it really needed? Pick your measurements very carefully, beamtime is limited and precious, *its your Thesis!*)

- Sample area: Count time scales linearly with area

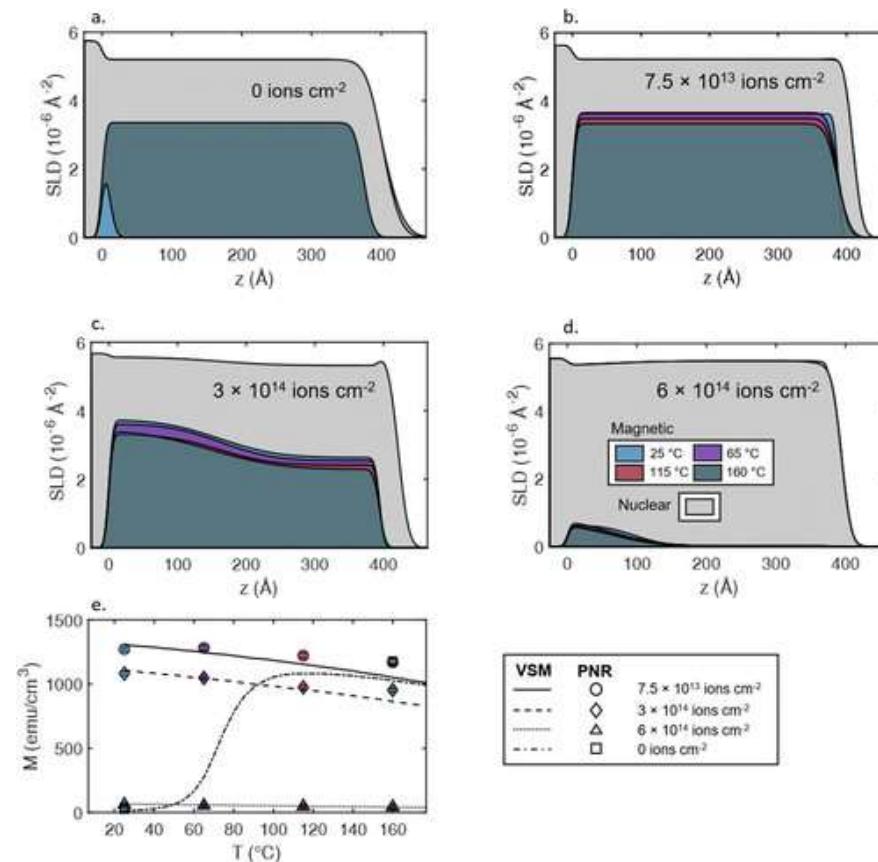
- SM samples sizes tend to by 80mm x 50 mm in area or bigger.
- PNR/PA samples tend to be 20 x 20 mm 10 x 10 mm or even 5 x 5 mm in area!
- A 20 x 20 mm sample will require a **factor 10** in count time to get the same level of statistics as an 80mm x 50mm SM Si block!
- **Point to take home for PNR/PA the larger the surface area the better!**

- Sample area: Other effects of small surface areas on data quality
  - Smaller Q range – its not possible to count out to high Q usually within the time allowed for an experiment.
  - Can you redesign your sample, not affecting the physics/chemistry/biology, to push the measurable effects to lower Q.
  - **Small sample often replace slit 2 as the final resolution optic! Think carefully about what resolution you need! This can have dramatic effects on resolution and count times!**
  - Tricks include:
    - Resonance effects
    - Bilayer/multilayering of the system to boost the signal into a Bragg peak.
    - Thick buffer/capping layers to shift the signal to lower Q in a radio carrier wave analogy.
    - Thickness variation of the various layers to make sure features of interest are not in intensity minima.
  - **When designing the experiment simulating the sample<sup>75</sup> and what you what to see is KEY to a successful experiment!**

# PNR/PA Practical points for experiments:

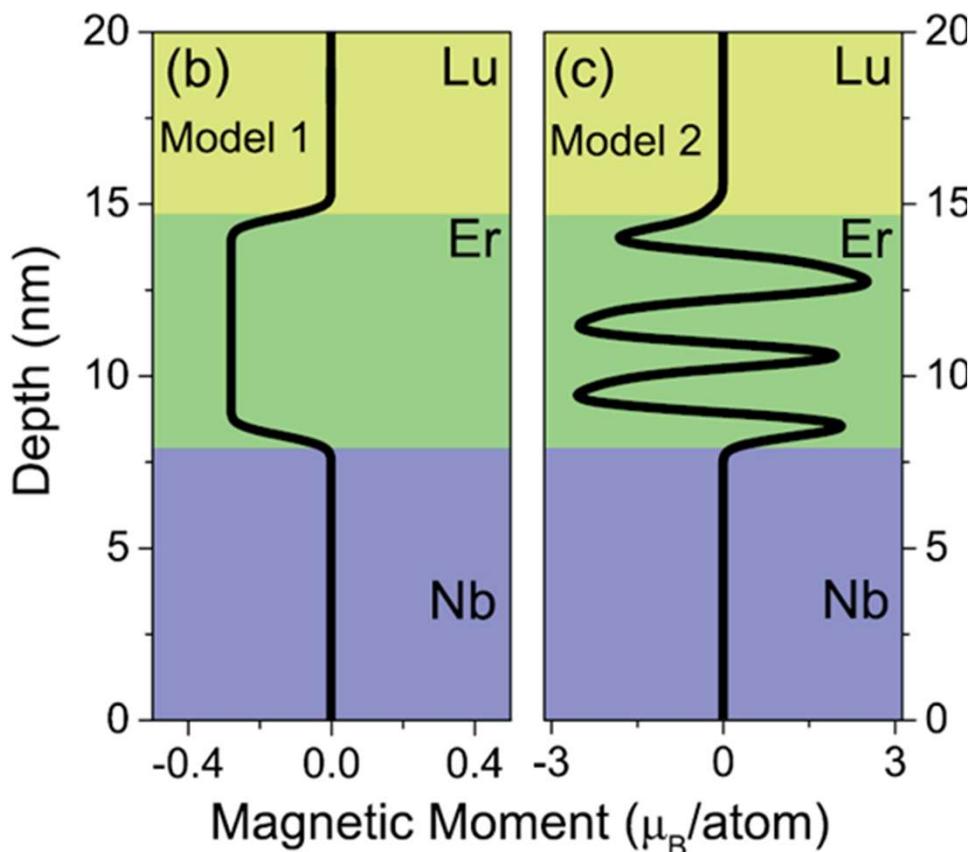
- Contrast is key for HCM

- Like in SM, HCM experiments need to think about contrasts.
- Trying to fit one PNR data set in isolation is very difficult as can get multiple solutions.
- If possible measure at  $H_{\text{sat}}$  and  $H_{\text{rem}}$  or at any other magnetic fields of interest and simultaneously fit the data.
- This also works if there is a variation of  $M$  in the sample with temperature.
- Measuring multiple fields or temperatures and fitting simultaneously is analogous to solving a simultaneous equations. This can vastly reduce ambiguity! (more in the lectures to come on this)



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# PNR/PA Practical points for experiments:



- **Null Experiments:**

- Often results are not clear, so think carefully about the null measurements you need to make to demonstrate an effect is present or not!
  - E.g. saturate the sample
  - E.g. change the temperature to be above or below a transition temperature.
- Experiment time is limited so pick carefully!
- Same idea applies to analysis of the data!

- **Setup time and correction/calibration measurements:**

- Remember to factor in any transmission measurements. **This is very important for SM experiments as not all Si blocks, etc are the same and may have different transmissions!**
- Remember to factor in sample environment changes like sample changes, sample alignment warm up and cool down times for cryostats
- **TALK TO THE LOCAL CONTACT ABOUT THE ABOVE!!!!!!**

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# PNR/PA Practical points for experiments:

- Pre characterise samples:
  - Please **Please** pre characterise your samples if at all possible! We have the R53 facility to help with this!
    - XRR at a bar minimum SQUID (HvsT or MvsT)
    - XRD/Transport/AFM/MOKE/TEM if you have time.
- Why? PNR/PA takes a long time to count out so you have to count in the right place on the right sample!
  - Does the sample display the effect/phenomena?
  - It is the worst idea in the world to use a PNR beamline like a SQUID because you don't know where the transition is. You could have just used a squid and be counting out the magnetic depth profile or vector profile which is what PNR/PA does best!
- The Mark 1 Eyeball is a good technique to use to check a sample is optically flat. I.e. if the sample is rough visibly! Its unlikely to work on a reflectometer!

- Pre characterise samples:
  - Anisotropies! Do you know the sample anisotropies, easy and hard axes?
  - SQUID/MOKE/crystallography
  - This is so the sample can be mounted in the right direction in the beamline.
- Silicon block roughness/substrate roughness! **THIS IS VERY IMPORTANT FOR SM experiments!** A quick XRR scan can show if you have a smooth block or not! If its too rough it will not work.

**In science fortune  
favours the prepared!**

# PNR/PA Practical points for experiments:

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# Useful slides



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## Useful Websites:

Need to calculate SLD's these will help:

- NIST SLD calculator: <http://www.ncnr.nist.gov/resources/activation/> (Neutron and x-ray scattering lengths)
  - NIST Table of scattering lengths and Cross sections: <http://www.ncnr.nist.gov/resources/n-lengths/>
  - ISIS Biomolecular Scattering Length Density Calculator: <http://psldc.isis.rl.ac.uk/Psldc/> For all your protein and peptide SLD needs. Also has a manual explaining how this is done!
  - NIST Resources including SANS and NR calculators: <http://www.ncnr.nist.gov/resources/>
  - WebElements: <http://www.webelements.com/> (Probably one of the most useful website on the web in my opinion)
  - X-ray interactions with Matter CXRO : [http://henke.lbl.gov/optical\\_constants/](http://henke.lbl.gov/optical_constants/)

NIST Center for Neutron Research		Neutron scattering lengths and cross sections													
Home	ICF	Experiments				UserProposal				Instruments				SiteMap	
Neutron scattering lengths and cross sections															
H	D	T	$\alpha$	$\mu$	$\pi^+$	$\pi^-$	$\pi^0$	$\rho$	$\eta$	$\sigma$	$\delta$	$\chi$	$\psi$		
He	$^{3\alpha}$	$^{4\alpha}$	$^{12}C$	$^{14}N$	$^{16}O$	$^{18}F$	$^{20}Ne$	$^{22}Mg$	$^{24}Si$	$^{26}S$	$^{28}Si$	$^{30}Si$	$^{32}S$	$^{34}S$	
$^{19}F$	$^{21}Ne$	$^{23}Na$	$^{25}Mg$	$^{27}Al$	$^{29}Si$	$^{31}P$	$^{33}S$	$^{35}Cl$	$^{37}Ar$	$^{39}K$	$^{41}Ca$	$^{43}Cr$	$^{45}Ti$	$^{47}V$	
$^{87}Rb$	$^{89}Sr$	$^{91}Y$	$^{93}Zr$	$^{95}Nb$	$^{97}Ta$	$^{99}Ru$	$^{101}Rh$	$^{103}Pd$	$^{105}Ag$	$^{107}Cd$	$^{109}In$	$^{111}Sn$	$^{113}Sb$	$^{115}Te$	
$^{133}Cs$	$^{135}Ba$	$^{137}La$	$^{139}Ce$	$^{141}Pr$	$^{143}Nd$	$^{145}Eu$	$^{147}Gd$	$^{149}Dy$	$^{151}Ho$	$^{153}Er$	$^{155}Tm$	$^{157}Yb$	$^{159}Lu$	$^{161}Hf$	
$^{171}Tm$	$^{173}Ho$	$^{175}Er$	$^{177}Tb$	$^{179}Dy$	$^{181}Yb$	$^{183}Lu$	$^{185}Hf$	$^{187}Tl$	$^{189}W$	$^{191}Re$	$^{193}Os$	$^{195}Pt$	$^{197}Au$	$^{199}Hg$	
$^{203}Tl$	$^{205}Bi$	$^{207}Po$	$^{209}At$	$^{211}Fr$	$^{213}Ra$	$^{215}Ac$	$^{217}Th$	$^{219}Pa$	$^{221}U$	$^{223}Ra$	$^{225}Ac$	$^{227}Fr$	$^{229}Rb$	$^{231}Fr$	
$^{233}Th$	$^{235}U$	$^{237}Np$	$^{239}Pu$	$^{241}Am$	$^{243}Cm$	$^{245}Bk$	$^{247}Cf$	$^{249}Bk$	$^{251}Cf$	$^{253}Bk$	$^{255}Cf$	$^{257}Bk$	$^{259}Cf$	$^{261}Bk$	
$^{289}Fl$	$^{291}Ra$	$^{293}Ac$	$^{295}Fr$	$^{297}Rb$	$^{299}Cs$	$^{301}Ba$	$^{303}La$	$^{305}Ce$	$^{307}Pr$	$^{309}Nd$	$^{311}Eu$	$^{313}Gd$	$^{315}Dy$	$^{317}Ho$	
$^{319}Tl$	$^{321}Bi$	$^{323}Po$	$^{325}At$	$^{327}Fr$	$^{329}Ra$	$^{331}Ac$	$^{333}Th$	$^{335}Pa$	$^{337}U$	$^{339}Ra$	$^{341}Ac$	$^{343}Fr$	$^{345}Rb$	$^{347}Cs$	
$^{361}Tl$	$^{363}Bi$	$^{365}Po$	$^{367}At$	$^{369}Fr$	$^{371}Ra$	$^{373}Ac$	$^{375}Th$	$^{377}Pa$	$^{379}U$	$^{381}Ra$	$^{383}Ac$	$^{385}Fr$	$^{387}Rb$	$^{389}Cs$	
$^{391}Tl$	$^{393}Bi$	$^{395}Po$	$^{397}At$	$^{399}Fr$	$^{401}Ra$	$^{403}Ac$	$^{405}Th$	$^{407}Pa$	$^{409}U$	$^{411}Ra$	$^{413}Ac$	$^{415}Fr$	$^{417}Rb$	$^{419}Cs$	
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$^{471}Tl$	$^{473}Bi$	$^{475}Po$	$^{477}At$	$^{479}Fr$	$^{481}Ra$	$^{483}Ac$	$^{485}Th$	$^{487}Pa$	$^{489}U$	$^{491}Ra$	$^{493}Ac$	$^{495}Fr$	$^{497}Rb$	$^{499}Cs$	
$^{521}Tl$	$^{523}Bi$	$^{525}Po$	$^{527}At$	$^{529}Fr$	$^{531}Ra$	$^{533}Ac$	$^{535}Th$	$^{537}Pa$	$^{539}U$	$^{541}Ra$	$^{543}Ac$	$^{545}Fr$	$^{547}Rb$	$^{549}Cs$	
$^{571}Tl$	$^{573}Bi$	$^{575}Po$	$^{577}At$	$^{579}Fr$	$^{581}Ra$	$^{583}Ac$	$^{585}Th$	$^{587}Pa$	$^{589}U$	$^{591}Ra$	$^{593}Ac$	$^{595}Fr$	$^{597}Rb$	$^{599}Cs$	
$^{621}Tl$	$^{623}Bi$	$^{625}Po$	$^{627}At$	$^{629}Fr$	$^{631}Ra$	$^{633}Ac$	$^{635}Th$	$^{637}Pa$	$^{639}U$	$^{641}Ra$	$^{643}Ac$	$^{645}Fr$	$^{647}Rb$	$^{649}Cs$	
$^{671}Tl$	$^{673}Bi$	$^{675}Po$	$^{677}At$	$^{679}Fr$	$^{681}Ra$	$^{683}Ac$	$^{685}Th$	$^{687}Pa$	$^{689}U$	$^{691}Ra$	$^{693}Ac$	$^{695}Fr$	$^{697}Rb$	$^{699}Cs$	
$^{721}Tl$	$^{723}Bi$	$^{725}Po$	$^{727}At$	$^{729}Fr$	$^{731}Ra$	$^{733}Ac$	$^{735}Th$	$^{737}Pa$	$^{739}U$	$^{741}Ra$	$^{743}Ac$	$^{745}Fr$	$^{747}Rb$	$^{749}Cs$	
$^{771}Tl$	$^{773}Bi$	$^{775}Po$	$^{777}At$	$^{779}Fr$	$^{781}Ra$	$^{783}Ac$	$^{785}Th$	$^{787}Pa$	$^{789}U$	$^{791}Ra$	$^{793}Ac$	$^{795}Fr$	$^{797}Rb$	$^{799}Cs$	
$^{821}Tl$	$^{823}Bi$	$^{825}Po$	$^{827}At$	$^{829}Fr$	$^{831}Ra$	$^{833}Ac$	$^{835}Th$	$^{837}Pa$	$^{839}U$	$^{841}Ra$	$^{843}Ac$	$^{845}Fr$	$^{847}Rb$	$^{849}Cs$	
$^{871}Tl$	$^{873}Bi$	$^{875}Po$	$^{877}At$	$^{879}Fr$	$^{881}Ra$	$^{883}Ac$	$^{885}Th$	$^{887}Pa$	$^{889}U$	$^{891}Ra$	$^{893}Ac$	$^{895}Fr$	$^{897}Rb$	$^{899}Cs$	
$^{921}Tl$	$^{923}Bi$	$^{925}Po$	$^{927}At$	$^{929}Fr$	$^{931}Ra$	$^{933}Ac$	$^{935}Th$	$^{937}Pa$	$^{939}U$	$^{941}Ra$	$^{943}Ac$	$^{945}Fr$	$^{947}Rb$	$^{949}Cs$	
$^{971}Tl$	$^{973}Bi$	$^{975}Po$	$^{977}At$	$^{979}Fr$	$^{981}Ra$	$^{983}Ac$	$^{985}Th$	$^{987}Pa$	$^{989}U$	$^{991}Ra$	$^{993}Ac$	$^{995}Fr$	$^{997}Rb$	$^{999}Cs$	

**NOTE:** The above are only thermal neutron cross sections. I do not have any energy dependent cross sections. For energy dependent cross sections please go to the National Nuclear Data Center at Brookhaven National Lab.

NIST Center for Neutron Research		NIST National Institute of Standards and Technology																									
<a href="#">Home</a>	<a href="#">Instruments</a>	<a href="#">Science</a>																									
<a href="#">Experiments</a>	<a href="#">SiteMap</a>																										
<p><b>Material</b>  <input type="text" value="Co"/></p> <p><b>Neutron Activation</b></p> <table border="1"> <tr> <td>Thermal flux</td> <td>Cd ratio</td> <td>For rabbit system</td> <td><input type="button" value="Calculate"/></td> </tr> <tr> <td>1e8</td> <td>0</td> <td>0</td> <td></td> </tr> <tr> <td>Mass</td> <td>Time on beam</td> <td>Time off beam</td> <td></td> </tr> <tr> <td>1</td> <td>10</td> <td>1y</td> <td></td> </tr> </table> <p><b>Absorption and Scattering</b></p> <table border="1"> <tr> <td>Density</td> <td>Thickness</td> <td><input type="button" value="Calculate"/></td> </tr> <tr> <td>Source neutrons</td> <td>Source X-rays</td> <td></td> </tr> <tr> <td>1 Ang</td> <td>Cu Ka</td> <td></td> </tr> </table>			Thermal flux	Cd ratio	For rabbit system	<input type="button" value="Calculate"/>	1e8	0	0		Mass	Time on beam	Time off beam		1	10	1y		Density	Thickness	<input type="button" value="Calculate"/>	Source neutrons	Source X-rays		1 Ang	Cu Ka	
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<p><b>Neutron activation and scattering calculator</b></p> <p>This calculator uses neutron cross sections to compute activation on the sample given the mass in the sample and the time in the beam, or to perform scattering calculations for the neutrons which are not absorbed by the sample.</p> <ol style="list-style-type: none"> <li>Enter the sample formula in the material panel.</li> <li>To perform activation calculations, fill in the thermal flux, the mass, the time on and off the beam, then press the calculate button in the neutron activation panel.</li> <li>To perform scattering calculations, fill in the wavelength of the neutron and/or x-rays, the thickness and the density (if not given in the formula), then press the calculate button in the absorption and scattering panel.</li> </ol>																											

# How to Calculate a Nuclear Scattering Length Density (nSLD)

- How do we calculate the SLD?
  - Easiest method: go to [www.ncnr.nist.gov/resources/sldcalc.html](http://www.ncnr.nist.gov/resources/sldcalc.html)
- By hand: let us calculate the scattering length density for quartz –  $\text{SiO}_2$ 
  - Density ( $\rho$ ) of  $\text{SiO}_2$  is  $2.66 \text{ gm.cm}^{-3}$ ; Molecular weight ( $M$ ) is  $60.08 \text{ gm. mole}^{-1}$
  - Number of molecules per  $\text{\AA}^3 = N$  is given by:

$$N = 10^{-2} \left( \frac{\rho}{M} \right) * N_{\text{Avagadro}}$$

$$N_{\text{Avagadro}} = 6.022 \times 10^{23}$$

$$N = 10^{-24} (2.66/60.08) * N_{\text{Avagadro}} = 0.0267 \text{ molecules per } \text{\AA}^3$$

$$SLD = Nb = N \sum b = \frac{\sum b}{Volume} = N(b_{\text{Si}} + 2b_{\text{O}})$$

$$\begin{aligned} \bullet SLD &= \sum b / \text{volume} = N(b_{\text{Si}} + 2b_{\text{O}}) = 0.0267(4.15 + 11.6) 10^{-5} \text{\AA}^{-2} \\ &= 4.21 \times 10^{-6} \text{\AA}^{-2} \end{aligned}$$

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# How to Calculate a Magnetic Scattering Length Density (mSLD)

- How do we calculate the SLD?
  - Easiest method: go to [www.ncnr.nist.gov/resources/sldcalc.html](http://www.ncnr.nist.gov/resources/sldcalc.html)
- By hand: first calculate the Nuclear scattering length density for saturated Ni -
  - Density ( $\rho$ ) of Ni is 8.908 gm.cm<sup>-3</sup>; Molecular weight ( $M$ ) is 58.69 gm. mole<sup>-1</sup>
  - Number of molecules per Å<sup>3</sup> =  $N$  is given by:

$$N = 10^{-24} \left( \frac{\rho}{M} \right) * N_{\text{avagadro}}$$

$$N_{\text{avagadro}} = 6.022 \times 10^{23}$$

$$N = 10^{-24} (8.908 / 58.6934) * N_{\text{avagadro}} = 0.0914 \text{ Ni atoms per } \text{\AA}^3$$

$$SLD = Nb = N \sum b = \frac{\sum b}{Volume} = N(b_{Ni})$$

$$b_{Ni} = 10.3 \text{ fm}$$

$$\bullet SLD = \sum b / volume = N(b_{Ni}) = 0.0914 * (10.3) * 10^{-5} \text{ \AA}^{-2} \quad (\text{the } *10^{-5} \text{ converts fm to \AA})$$

$$SLD_{Ni} = 9.41 \times 10^{-6} \text{ \AA}^{-2}$$

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# How to Calculate a Magnetic Scattering Length Density (mSLD)

- The saturated total magnetic moment of Ni is  $0.6 \mu_b/\text{atom}$  which is equivalent to approximately  $508 \text{ emu/cm}^3$  as would be measured by a magnetometer.
- The magnetic component of the SLD is given by:

$$SLD_M = \sum_i^J N_i b_{mi} = C \sum_i^J N_i \mu_i = Cm$$

- The units of the magnetic scattering length,  $b_m$ , are  $\text{\AA}$ . This is the magnetic equivalent to the nuclear scattering length  $b$ , denoted  $b_N$ .
- The magnetic moment per formula unit,  $\mu$ , is in units of Bohr magnetons  $\mu_B$ 
  - In this case the constant is  $C = 2.645 \times 10^{-5} \text{\AA} \mu_B^{-1}$
- More usefully we normally measure the magnetisation  $M$  in a magnetometer and convert it to magnetic moment  $m$  by dividing it by the sample volume.
  - If  $m$  is in units of Tesla, then  $C = 2.645 \times 10^{-5} / 4\pi \text{\AA}^2 \text{T}^{-1}$
  - If  $m$  is in units of  $\text{emu}/\text{cm}^3$ , then  $C = 2.853 \times 10^{-9} \text{\AA}^2 \text{cm}^3 \text{emu}^{-1}$

This is taken from "Application of polarized neutron reflectometry to studies of artificially structured magnetic materials" by M. R. Fitzsimmons and C. F. Majkzak

## How to Calculate a Magnetic Scattering Length Density (mSLD)

$$\text{SLD}_m = \pm C N_i \mu_i = \pm 2.645 \times 10^{-5} \times 0.0914 \times 0.6 = \pm 1.451 \times 10^{-6} \text{ \AA}^{-2}$$

- The following from what we know about the SLD's:

$$\text{SLD}_{\text{Ni}} = \text{SLD}_{\text{Ni (Nuclear)}} \pm \text{SLD}_{\text{Ni (Magnetic)}}$$

$$\begin{aligned}\text{SLD}_{\text{Ni+}} &= (9.41 + 1.451) \times 10^{-6} \text{ \AA}^{-2} = 10.861 \times 10^{-6} \text{ \AA}^{-2} \\ \text{SLD}_{\text{Ni-}} &= (9.41 - 1.451) \times 10^{-6} \text{ \AA}^{-2} = 7.959 \times 10^{-6} \text{ \AA}^{-2}\end{aligned}$$

- This results in two very independent reflectivity curves each with their own critical edge
- This is what is measured by the Up and Down spin state reflectivity curves.

**This is taken from “Application of polarized neutron reflectometry to studies of artificially structured magnetic materials” by M. R. Fitzsimmons and C. F. Majkzak**

# What kind of Scientific information can SANS tell you:

- A SANS beamline is a diffractometer optimized for small angles
- Works for length scales from 1 nm up to 1000nm which translates to very low  $Q \approx 1\text{\AA}^{-1}$  to  $10^{-4}\text{\AA}^{-1}$
- SANS tells you the Statistical average of:
  - Shape of the scattering object
  - Size (distribution) of the scattering objects
  - Surface of the scattering objects
  - Scattering length density (distribution)
  - Arrangement (Superstructure)

# What kind of Scientific information can PolSANS (Magnetic SANS is not POLSANS) tell you:

- Magnetism on the scale of 3nm to 300nm (The nanoscale)
- Magnetic SANS is not polarised SANS
  - Magnetic SANS is sensitive to the deviation of the mean magnetization:
- Use SANSPOL (half polarized) and POLARIS (full polarization analysis) for a full picture/ discrimination of SF/NSF scattering (comes at the price of intensity).



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# Thank you

[Christy.kinane@stfc.ac.uk](mailto:Christy.kinane@stfc.ac.uk)

# SAS measurements

## Plan your experiment well!

- What Q-range would I like, and what must I have?
  - How large is each sample?
  - How much material do I need?
  - For how long should I measure my samples?
  - How can I optimize my sample quality?
  - What control measurements do I need to perform?
  - How will I reduce my data?
- 
- Less is often more: Do fewer things but those do right! (especially with neutrons)

**Ask your local contact / instrument scientist for advice well ahead of time!**



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Tutorial Questions:

Converting SQUID data to emu/cm<sup>3</sup> and A/m:

Calculating mSLD's



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