Reflectometry Science away day:

What are we presenting in publications?

Or rather what should we suggest people present and how?

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The thing we do---- We need to display results in publications:

Objectives: All of these depend on the question/s you're trying to answer

1) *what should we suggest people put in the main paper and the SI?*
2) *What is the bare minimum we should put in the main paper and the SI?*
3) *What is what we feel is the recommended number of things to put in the main paper and SI?*

Ideally, we want to establish suggested best practices for SM/HCM as to what should be displayed in papers considering:

- *Experiments are all asking different questions.*
- *Improvements in analysis software – we can do more than ever before.*
- *Changing Journal Requirements*
- *Open data policies*
- ***Experimental reproducibility/replication***

The basic list of things we put in papers once the analysis is done

- Tables of Parameters with associated errors*# :
  - Useful but should only be in SI I feel
- Model descriptions*:
  - A lot of journals are asking for the data and fit files these days.
  - A description of the model and how it is constructed should be given at a minimum in the paper/SI
  - Priors:
    - Are the priors Uniform or Gaussian, etc
    - Max min values
- NR/PNR/PA Fits*:
  - need to show at least one example of fits done.
  - 95/98% confidence intervals
  - Spin Asymmetry plots for HCM
- SLD's*:
  - 95/98% confidence intervals
  - HCM magnetism profiles
  - No agreed upon way of showing PA profiles
  - SM profiles/ mag contrast
  - SM volume fraction plots
  - Absorption cross sections

- Distributions*:
  - Show them all, or only the ones for the important parameters?
  - Mean, Mode, Medium and best fit
- Correlation plots:
  - Corner plots get very big very quickly again maybe only show correlations on important parameters?
- Model selection/fitting method:
  - Chi^2 vs Parameter plots
  - Bayes evidence term plots
- Other things that need to be shown
  - Model 0 or zeroth order model to show the ideal case doesn't work.
  - Substrate characterisations – especially if used to constrain other models, arguable part of the fit but not shown.
  - Fitting methodology
- What other information to quote on how the model was fitted?
  - Fitting Software used
  - Figure of Merrit used? Chi^2 what are you using etc
  - Minimiser? MCMC, nested sampler, etc
  - **Residual plots? Help show where fitting isn't working like critical edges**
  - **What is the analysis meant to achieve? What questions will it answer?**

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I feel that the things in the red boxes constitute a set of the bare minimum.
This list is for specular data only!

Tables of Parameters with associated errors:

Taken from the SI of Awana *et. al.* Phys. Rev. Materials 6, 053402 – 2022
And the main text of Hall *et. al.* Biophysical Journal 120, 5295–5308, 2021 5301

- Useful, but detailed tables maybe in SI only?
- Use reduced versions in main text of important parameters
- Always quote errors with any values
- I find it a good exercise to make students etc make these tables to check their numbers aren't mental.

Questions:

- **When is this required or is it at all?**
- **How best to do this? (what to include)**
- **What level is appropriate?**
- **Should we include Max/Min priors?**
- **Where to put this , in SI/main text?**

TABLE 1 Structural parameters obtained by fitting PNR data of hBamA$^{(L7H9)}$BCDE/POPC membrane tethered to an Si-Py-Au-DTSP-ANTA-Cu^{2+} substrate

Layer	Thickness (Å)	Net SLD ($\times 10^{-6}$ Å^{-2})		Component volume fractions (%)		Roughness (Å)
Si	ND		2.07[a]	Si:	100[a]	$9.6^{+0.3}_{-0.6}$
SiO_2	$22.2^{+0.6}_{-0.5}$		$4.41^{+0.08}_{-0.12}$	SiO_2:	100[a]	$4.1^{+0.5}_{-0.5}$
Permalloy	$114.3^{+0.3}_{-0.2}$	↑:	$9.89^{+0.01}_{-0.01}$	Permalloy:	100[a]	$8.3^{+0.3}_{-0.3}$
		↓:	$7.22^{+0.01}_{-0.01}$			
Gold	$182.7^{+0.4}_{-0.3}$		4.62[a]	Gold:	100[a]	$5.9^{+0.1}_{-0.1}$
DTSP-ANTA-Cu^{2+} SAM	$9.8^{+1.3}_{-1.4}$		1.80[a]	DTSP-ANTA-Cu^{2+}:	56^{+8b}_{-6}	$4.6^{+1.7}_{-2.0}$
				Solvent:	44^{+6}_{-8}	
hBamA$^{(L7H9)}$BCDE (between SAM and membrane)	$31.2^{+1.6}_{-1.6}$	D_2O:	$3.08^{+2.17E-3b}_{-2.93E-3}$	hBamA$^{(L7H9)}$BCDE:	28^{+1b}_{-1}	$9.8^{+0.2}_{-0.3}$
		AuMW:	$2.78^{+0.43E-3b}_{-0.58E-3}$			
		PrMW:	$2.45^{+0.01b}_{-0.01}$	Solvent:	72^{+1}_{-1}	
		H_2O:	$2.05^{+0.05b}_{-0.02}$			
hBamA$^{(L7H9)}$BCDE + β-OG	$40.6^{+1.6}_{-1.7}$	D_2O:	$3.07^{+0.01b}_{-0.02}$	β-OG:	$0.2^{+0.3}_{-0.2}$	$9.8^{+0.2}_{-0.3}$
				hBamA$^{(L7H9)}$BCDE:	29^{+1b}_{-1}	
				Solvent:	71^{+1b}_{-1}	
hBamA$^{(L7H9)}$BCDE + POPC bilayer	$40.6^{+1.6}_{-1.7}$	D_2O:	$1.74^{+0.04b}_{-0.04}$	POPC:	26^{+1b}_{-1}	$9.8^{+0.2}_{-0.3}$
		AuMW:	$1.58^{+0.04b}_{-0.03}$	hBamA$^{(L7H9)}$BCDE:	29^{+1b}_{-1}	
		PrMW:	$1.41^{+0.03b}_{-0.03}$	Solvent:	45^{+1}_{-1}	
		H_2O:	$1.20^{+0.03b}_{-0.03}$			
hBamA$^{(L7H9)}$BCDE (adjacent to bulk solvent)	$84.4^{+7.1}_{-8.0}$	D_2O:	$3.08^{+2.17E-3b}_{-2.93E-3}$	hBamA$^{(L7H9)}$BCDE:	7^{+1b}_{-1}	$9.8^{+0.2}_{-0.3}$
		AuMW:	$2.78^{+0.43E-3b}_{-0.58E-3}$	Solvent:	93^{+1}_{-1}	
		PrMW:	$2.45^{+0.01b}_{-0.01}$			
		H_2O:	$2.05^{+0.02b}_{-0.02}$			
Bulk solvent	ND	D_2O:	$6.39^{+0.01}_{-0.02}$	Solvent:	100[a]	ND
		AuMW:	$4.70^{+2.39E-3}_{-3.25E-3}$			
		PrMW:	$2.84^{+0.06}_{-0.06}$			
		H_2O:	$0.62^{+0.10}_{-0.09}$			

Error values indicate the 95% confidence intervals estimated from MCMC resampling.
ND, not determinable.
[a]Values were held constant throughout the fitting procedure.
[b]Values were not directly fit, but calculated from the fitted parameters and associated 95% confidence intervals calculated from MCMC chains of the dependent fitted parameters.

Model 1: CrSe magnetism only						
Layer	Thickness (Å) ± 95% BI	Roughness (Å) ± 95% BI	Fitted nSLD $\times 10^{-6}$ Å^{-2} ± 95% BI	Bulk nSLD $\times 10^{-6}$ Å^{-2} ± 95% BI	Fitted mSLD $\times 10^{-6}$ Å^{-2} ± 95% BI	Equivalent magnetic moment μ_B/f.u.
Vacuum						
Surface layer	88 [65, 104]	70 [55, 87]	0.6 [0.4, 0.8]			
Bi_2Te_3	155.5 [154.6, 156.3]	12 [10, 14]	2.26 [2.21, 2.32]	2.01		
MnTe	320.9 [319.7, 322.1]	22.0 [20.7, 23.4]	0.42 [0.39, 0.45]	0.41		
CrSe 3 K	85.8 [84.7, 86.9]	0.64 [0.03, 1.80]	1.29 [1.27, 1.30]	3.6	0.24 [0.13, 60]	0.83 [0.45, 2.04]
CrSe 300 K	as 3 K	as 3 K	as 3 K	3.6	0.08 [-0.02, 0.6]	0.3 [-0.06, 2.06]
GaAs interface	4698 [4575, 4901]	0.52 [0.02, 1.47]	2.974 [2.973, 2.976]	3.07		
GaAs substrate		366 [298, 434]	fixed to bulk	3.072		

TABLE I. Model 1: All numbers without Bayesian uncertainty intervals (BI) were fixed. The starting density values were taken from the NCNR scattering database [8]. Please note that the numbers in square brackets are the Bayesian uncertainty intervals, which can be asymmetric. The values are quoted per formula unit (f.u.).

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Tables of Parameters with associated errors:

ACS Applied Materials & Interfaces www.acsami.org Research Article

Table 1. Summary of the PNR Results for the Rotated Graphene/Ni, Epitaxial Graphene/Ni, and Graphene/Ni_9Mo_1 Samples Using Model 16: Sapphire/FM Layer Split into Two Regions/Graphene[a]

		FM layer1 + FM layer2		graphene	
sample	temperature (K)	thickness (nm)	magnetic moment (μ_B/atom)	thickness (nm)	magnetic moment (μ_B/atom)
rotated Gr/Ni	10	82.8 (80.8, 82.8)	0.61 (0.61, 0.62)	0.82 (0.81, 1.2)	0.41 (0.28, 0.48)
	300		0.58 (0.57, 0.58)		0.23 (0.02, 0.41)
epitaxial Gr/Ni	10	77.4 (77.0, 77.6)	0.60 (0.60, 0.61)	0.99 (0.82, 1.2)	0.41 (0.25, 0.51)
	300		0.580 (0.576, 0.583)		0.15 (0.05, 0.46)
Gr/Ni_9Mo_1	10	77.1 (76.4, 77.7)	0.060 (0.056, 0.066)	1.0 (0.81, 1.2)	0.34 (0.06, 0.56)
	300		0.001 (−0.003, 0.006)		−0.01 (−0.04, 0.26)

[a]The top Ni layer and graphene roughnesses have been linked to make them conformal. The values in the parentheses are the lower and upper 95% Bayesian confidence limits.[62]

TABLE S3. Comparison of models 9, 14, 15 and 16. The values in the parenthesis are the lower and upper 95% Bayesian confidence limits.[27]

		FM Layer1 + FM Layer2		Graphene	
Model	Temperature [K]	Thickness [nm]	Magnetic moment [μ_B/atom]	Thickness [nm]	Magnetic moment [μ_B/atom]
Model 9	10 K 300 K	80.6(80.2,81.3)	0.60(0.60,0.61) 0.57(0.56,0.57)	0.86(0.81,1.04)	0.53(0.52,0.54) 0.53(0.51,0.54)
Model 14	10 K 300 K	82.7(81.4,83.7)	0.62(0.61,0.62) 0.58(0.57,0.58)	0.78(0.3,1.1)	0.48(0.16,0.52) 0.00(0.00,0.16)
Model 15	10 K 300 K	81.2(80.2,81.9)	0.60(0.60,0.61) 0.57(0.57,0.58)	0.82(0.81,1.16)	0.53(0.52,0.54) 0.51(0.47,0.53)
Model 16	10 K 300 K	82.8(80.8,82.8)	0.61(0.61,0.62) 0.58(0.57,0.58)	0.82(0.81,1.2)	0.41(0.28,0.48) 0.23(0.02,0.41)

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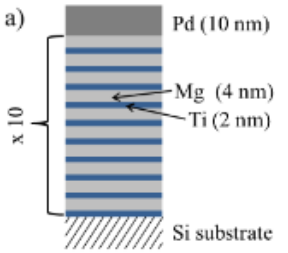
R. Aboljadayel *et. al.* ACS Appl. Mater. Interfaces 2023, 15, 18, 22367–22376

Model descriptions:

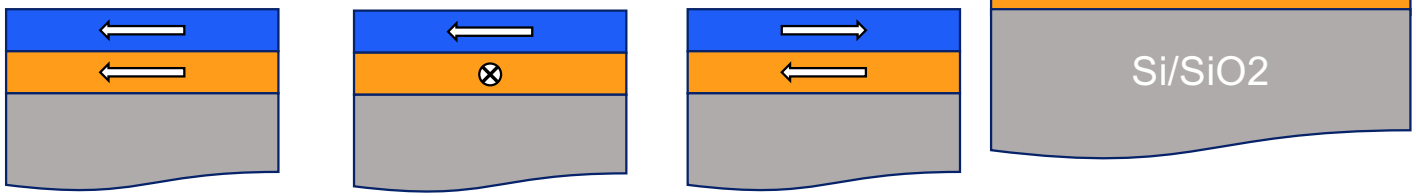
Some figures stolen from Leo et al (I asked permission)



- I normally do this in the text with a figure to aid?
  - A description of the model and how it is constructed should be given at a minimum in the paper/SI
  - Priors:
    - Are the priors Uniform or Gaussian, etc
    - Max min values and some information on how they were ascertained.

- A lot of journals are asking for the data and fit files these days to be stored on archives as part of open-access policies. Does this cover this ? I feel we need both for repeatability purposes/understanding

- Questions:
  - How best to do this?
  - How can we make this into a diagram maybe? (show layer model etc ? Fake SLD profile?
  - Magnetism often benefits form figure showing magnetic layer direction ?
  - Is this even worth doing for SM like this?



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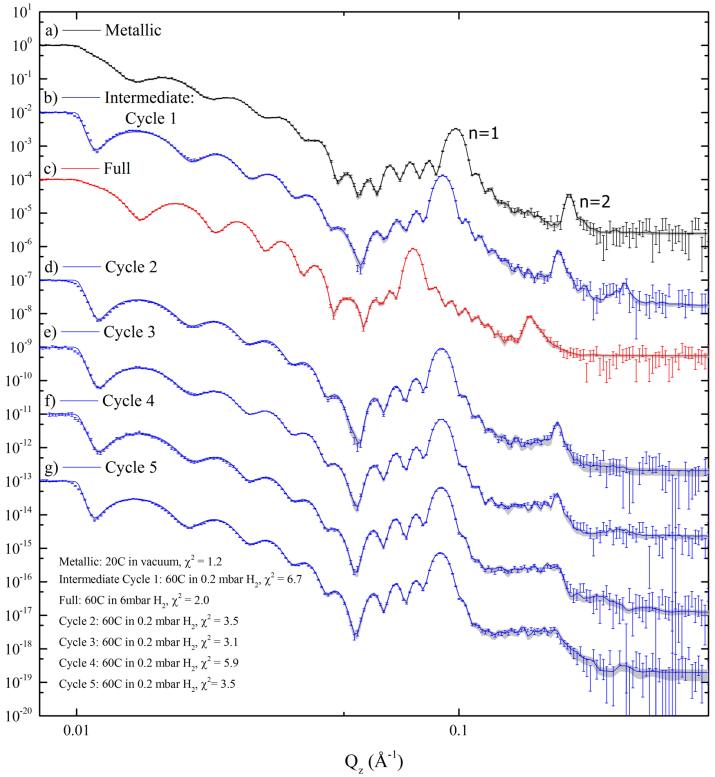
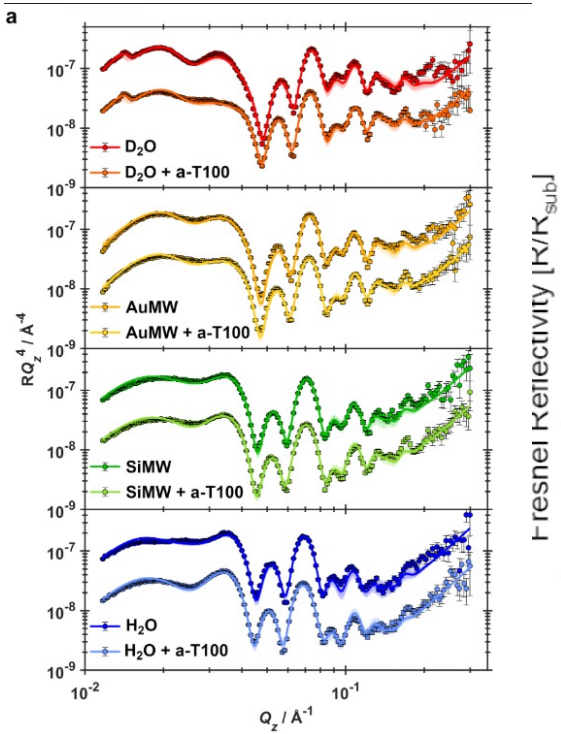
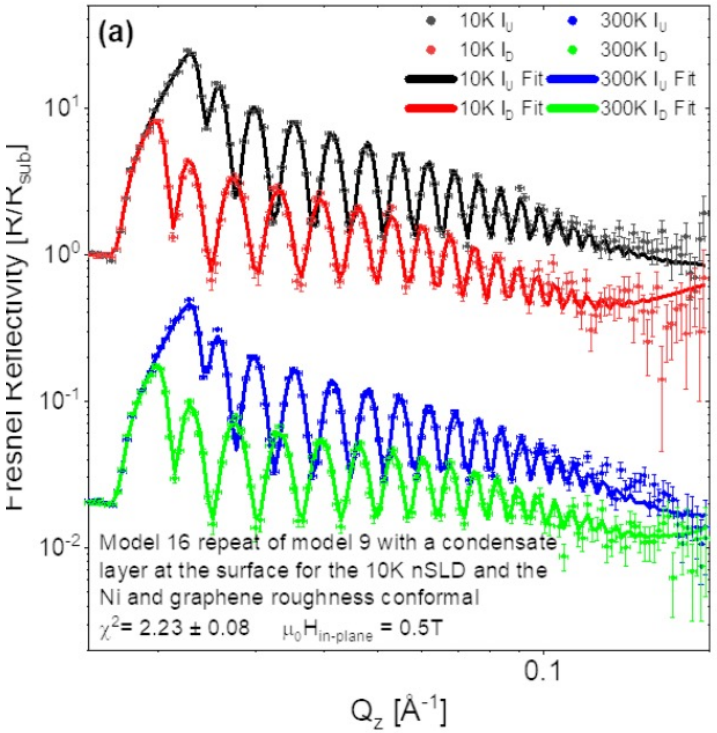
NR/PNR/PA fits

Data courtesy of Hall et al. and R. Aboljadayel et al



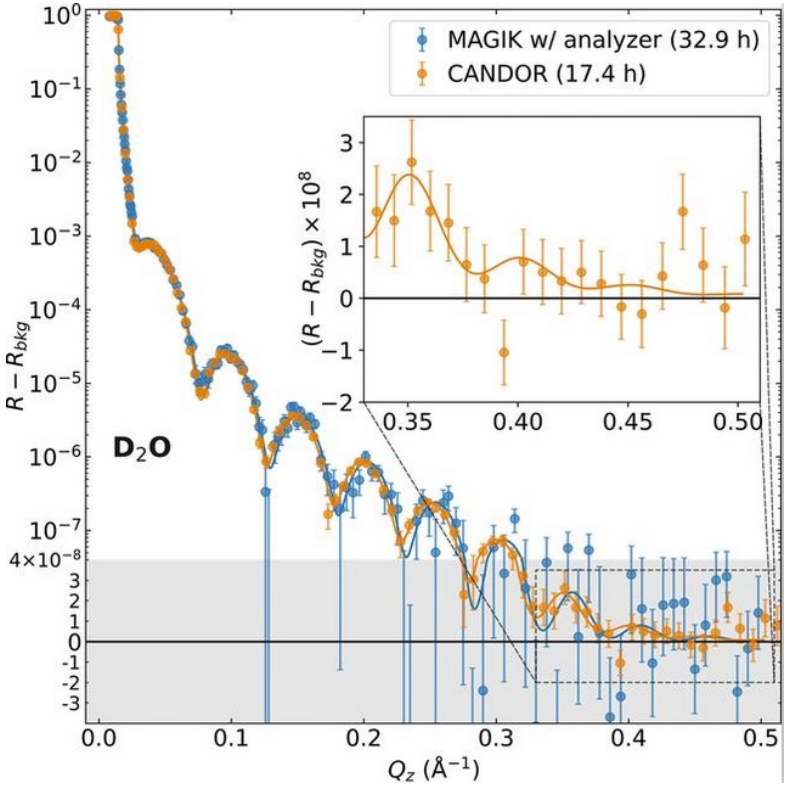




Some questions:

- Should you include 95% confidence intervals on these plots?
- How many curves do you need to show in main text or SI? Enough to show differences with SE conditions maybe?
- Indicate goodness of fits? Chi^2 displayed on plots
- Which is best Log/log, RQ4/log or R/Rsub/log ?

NR/PNR/PA data and Fits: what to do with negative data points from background subtraction



- First what do they mean?
- If we should dispalye them how do we do it?
- Example from David Hoogerheide . Appl. Cryst. (2022). 55, 58–66
- **What else is the bare minimum or recommended for main text or SI?**

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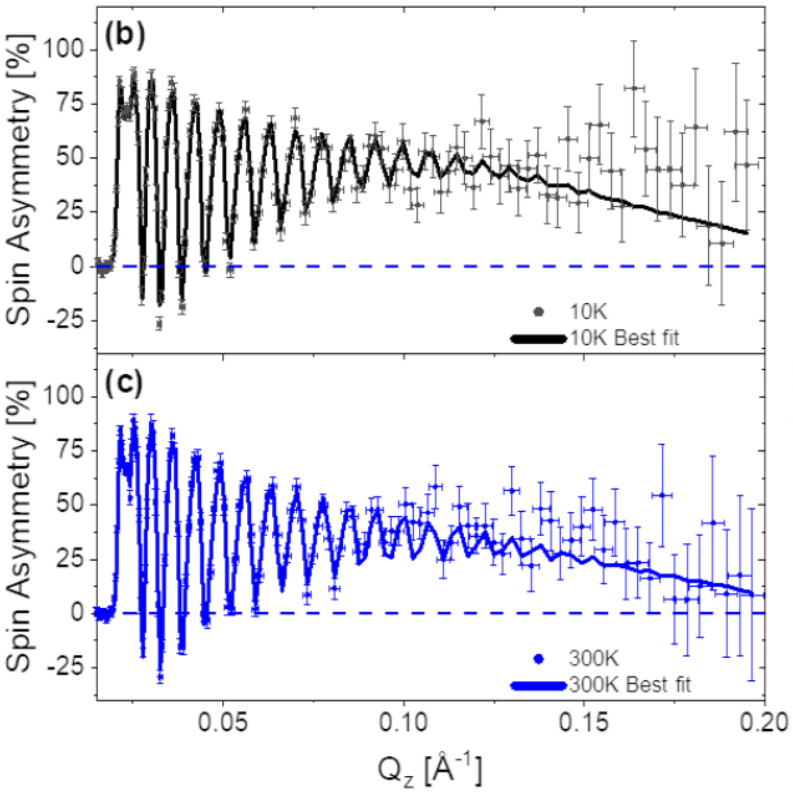
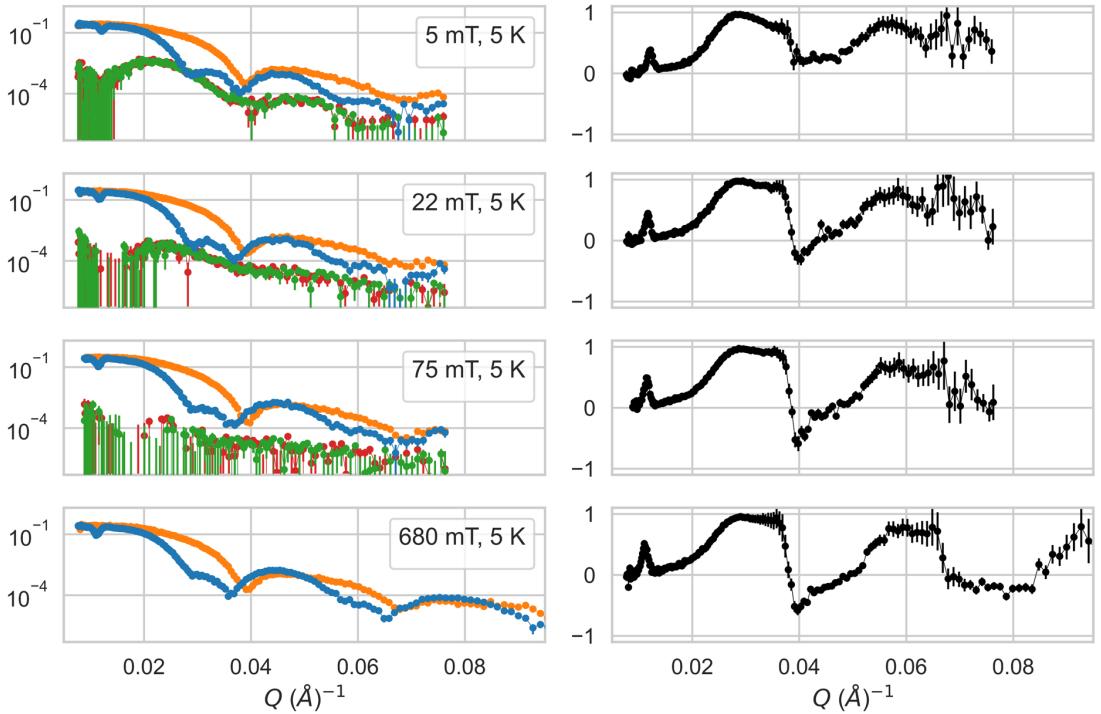
PNR/PA fits

PA data from Leo et al
SA form

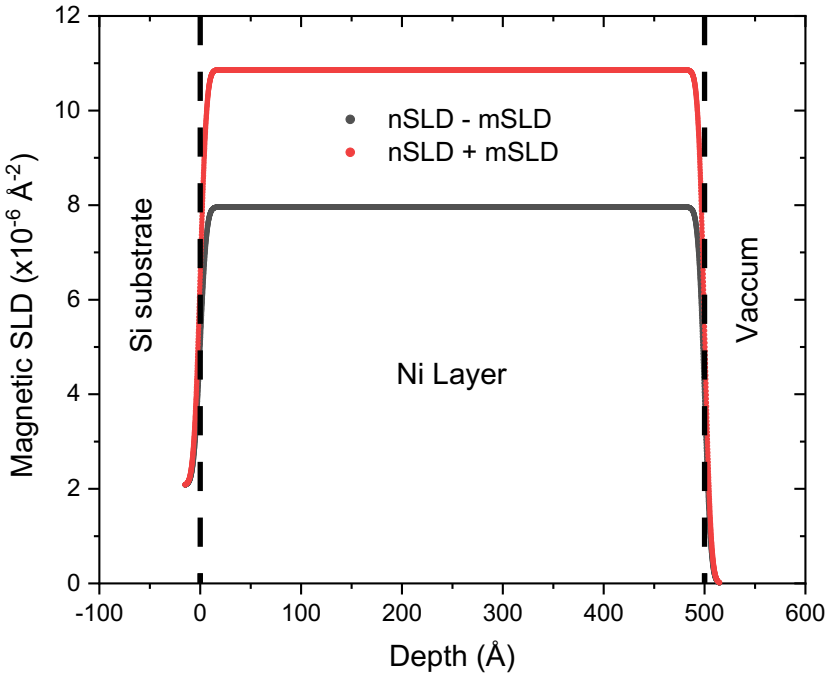


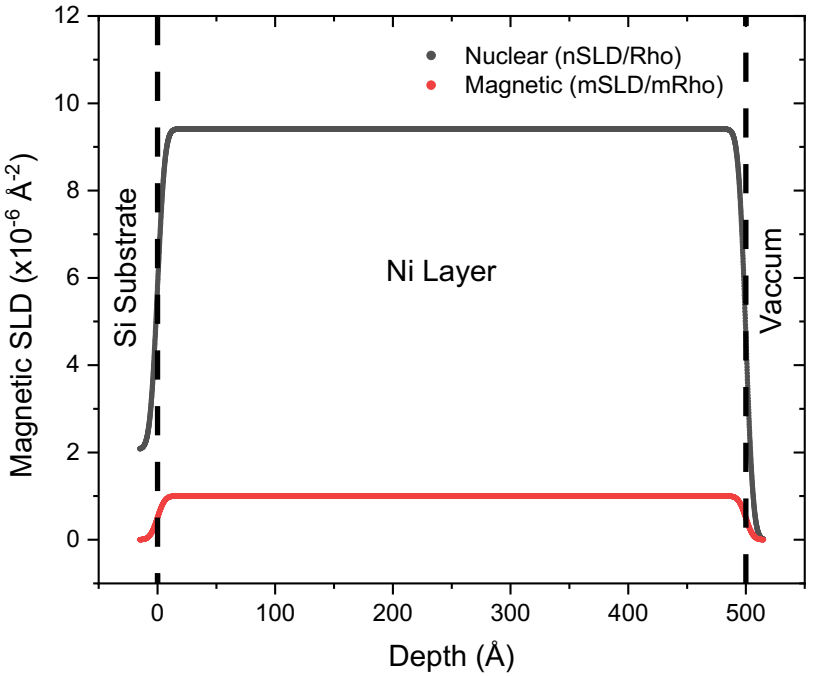


- Spin asymmetry, very useful for magnetism exp's needs defining in text of pubs
- PA data rarely seen in papers . POLREF now works well for it. Spin states need labelling for clarity
- We should probably show the PA sensitivity level some how? Like in proposals on sims?
- What else should we be displaying for HCM magnetism ?

SLD's: PNR/PA Practical points :

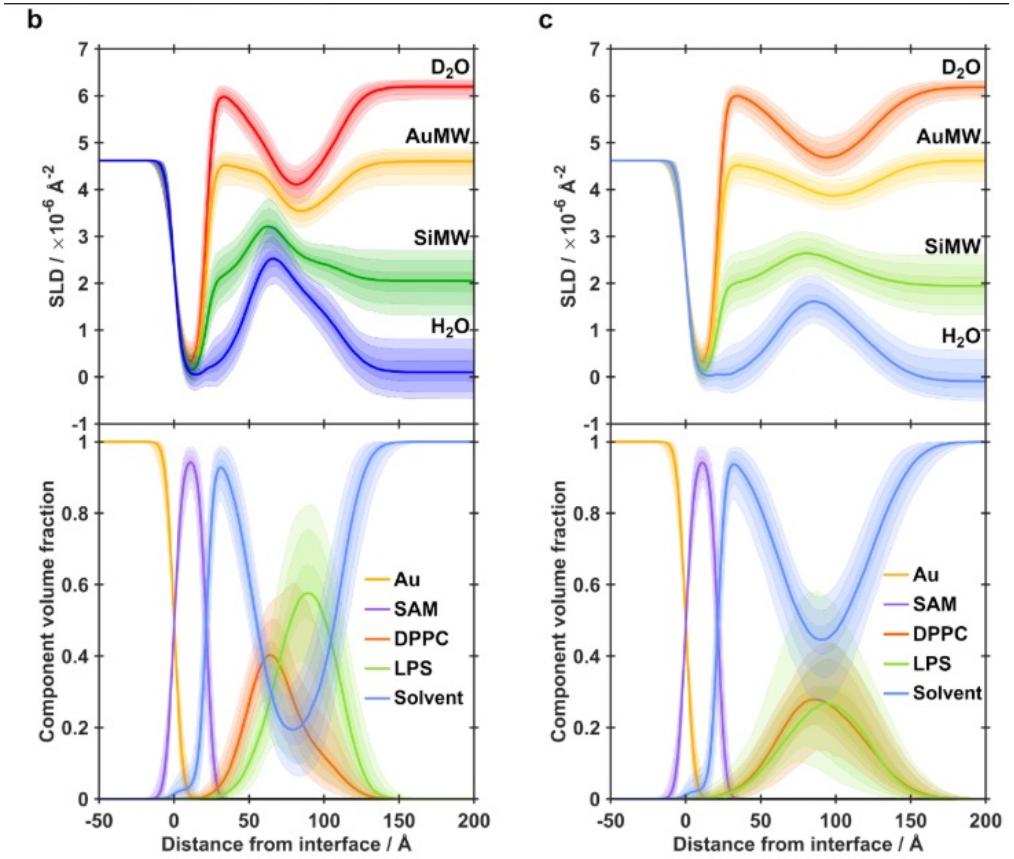
- Plotting PNR SLD profiles for Hard Condensed Matter (HCM) and Soft Matter (SM) experiments is different as they have different aims.

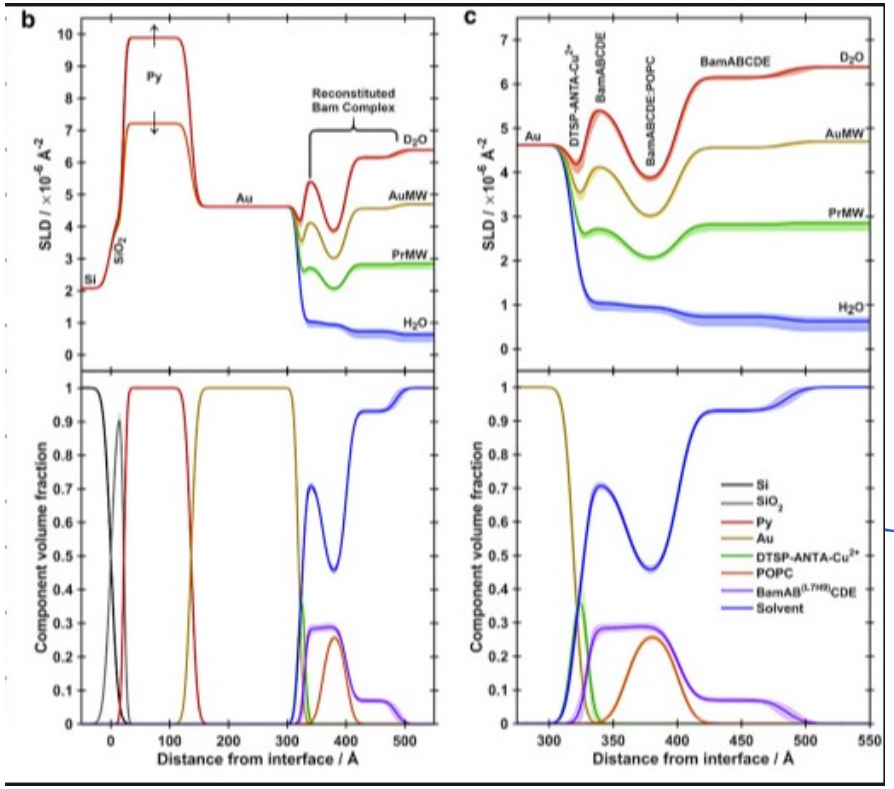




- LHS: In SM the mSLD is added to the nSLD as the magnetic profile is effectively irrelevant its just there to add another contrast. This is what the spin up and down neutrons actually interact with.
- RHS: In HCM the magnetic mSLD profile is the thing that is actually wanted so it is best to deconvolve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

SLD's for SM. Note SLD to my mind is most important thing to display.



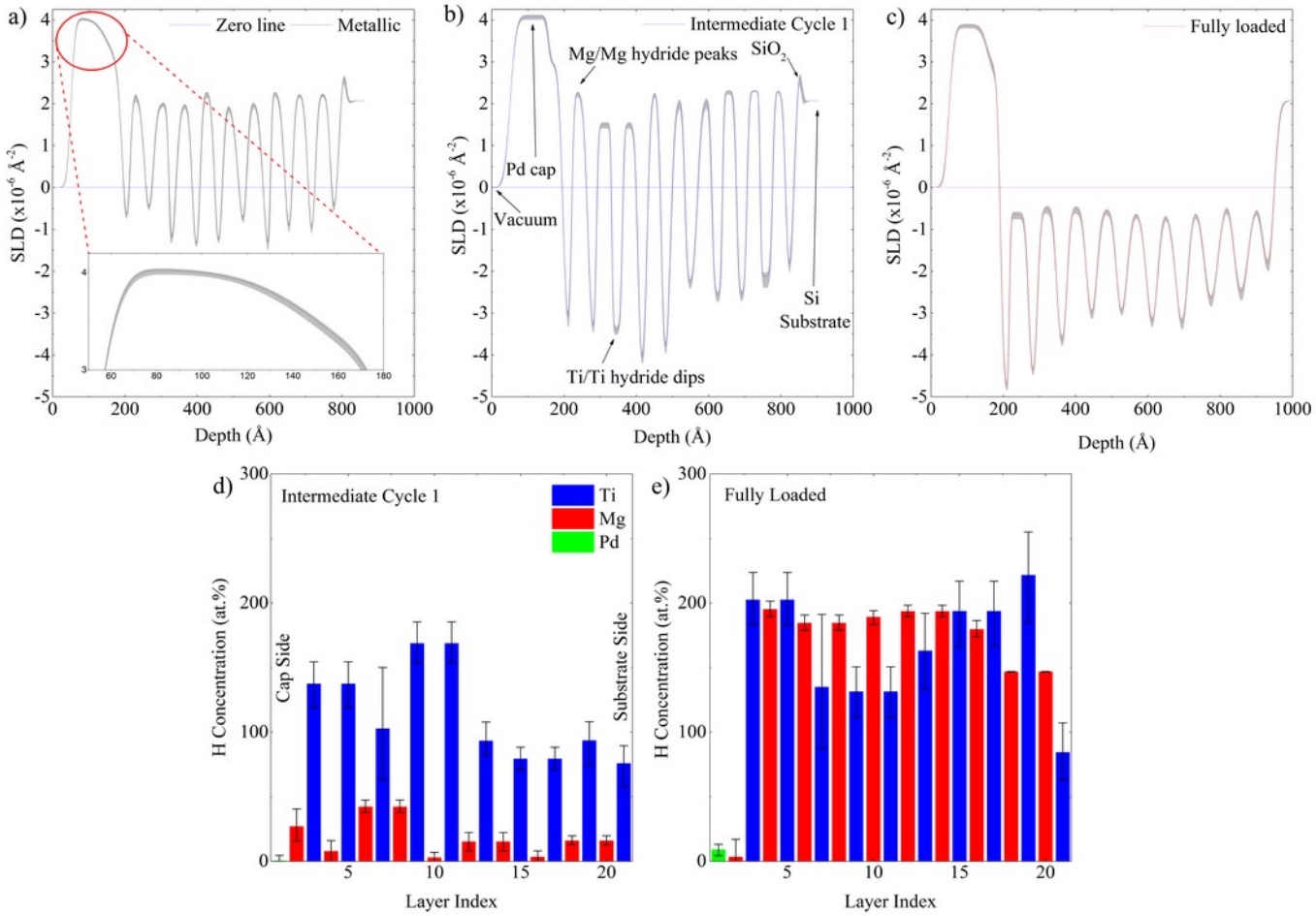


- 95% confidence intervals now very important
- Volume fraction may be more useful though for SM?
- Magnetism often displayed as two SLDs for soft matter.

Figures courtesy of Hall et al.

SLD's: Examples of non-magnetic hard matter

- Display Enough SLD's to show changes
- Figures where we extract other information from SLD's
- Would probably work with a volume fraction as well.



Kinane et al not published

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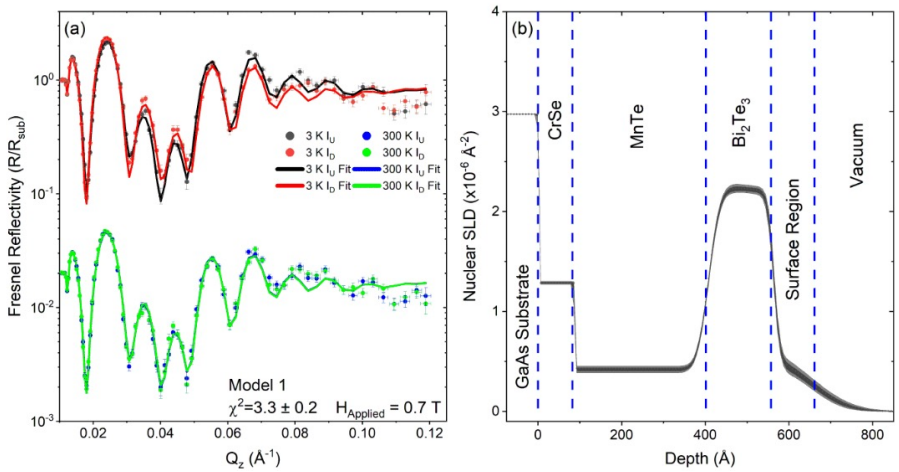
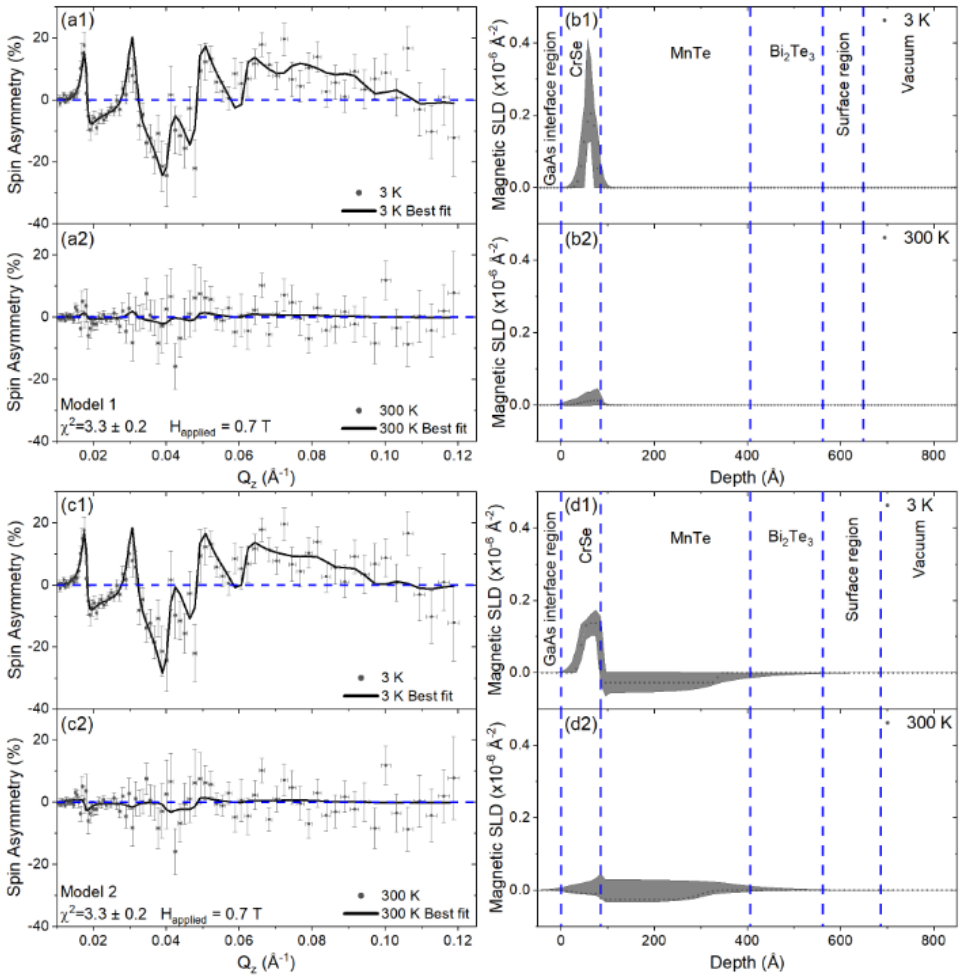
SLD's: PNR examples for HCM



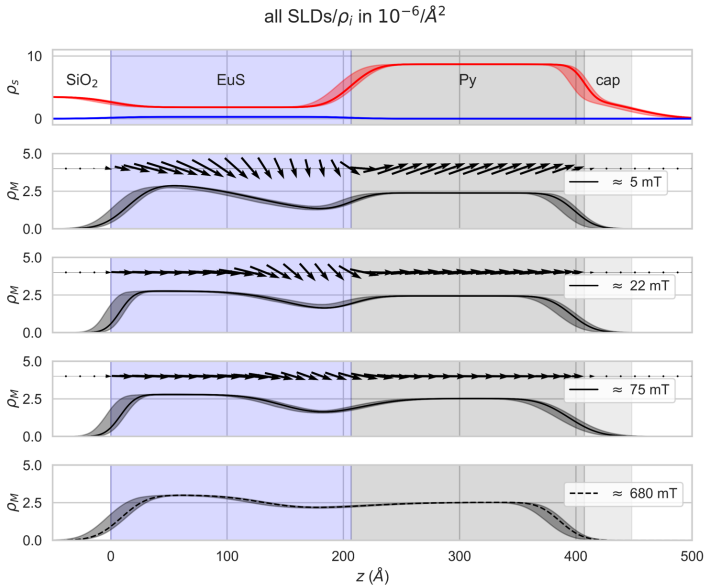


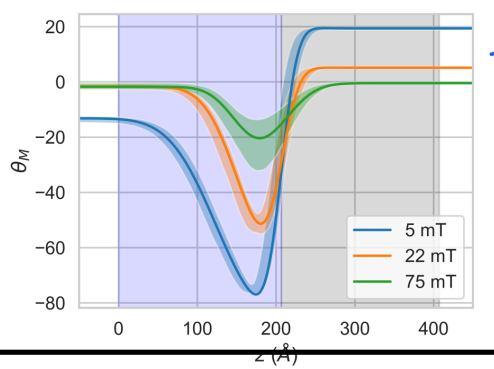
- An example of HCM from Awana et al
- Contrasts different fit models looking for Proximity induced magnetism (PIM) in topological insulators.
- 95% bounds critical for low signal magnetism work

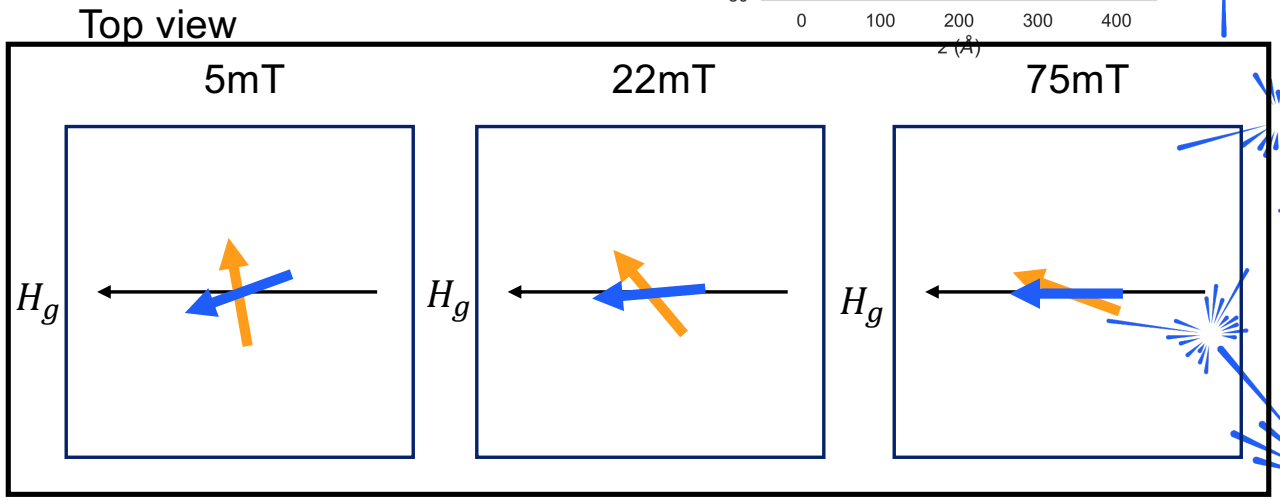
SLD's PA data plots: Not many examples in literature

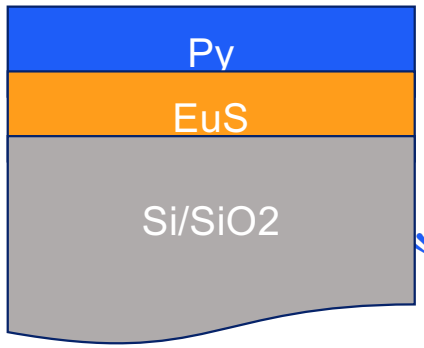
- Here is an example of what can be done

Again courtesy of Leo et al to be published









- More degrees of freedom than normal SLD plots
- Can be hard to visualise if your mind sees this as a standard SLD plot as its showing angle as that's more useful.
- Angle of M to P literally changes magnetic contrast so could just show multiple magnetic SLD's

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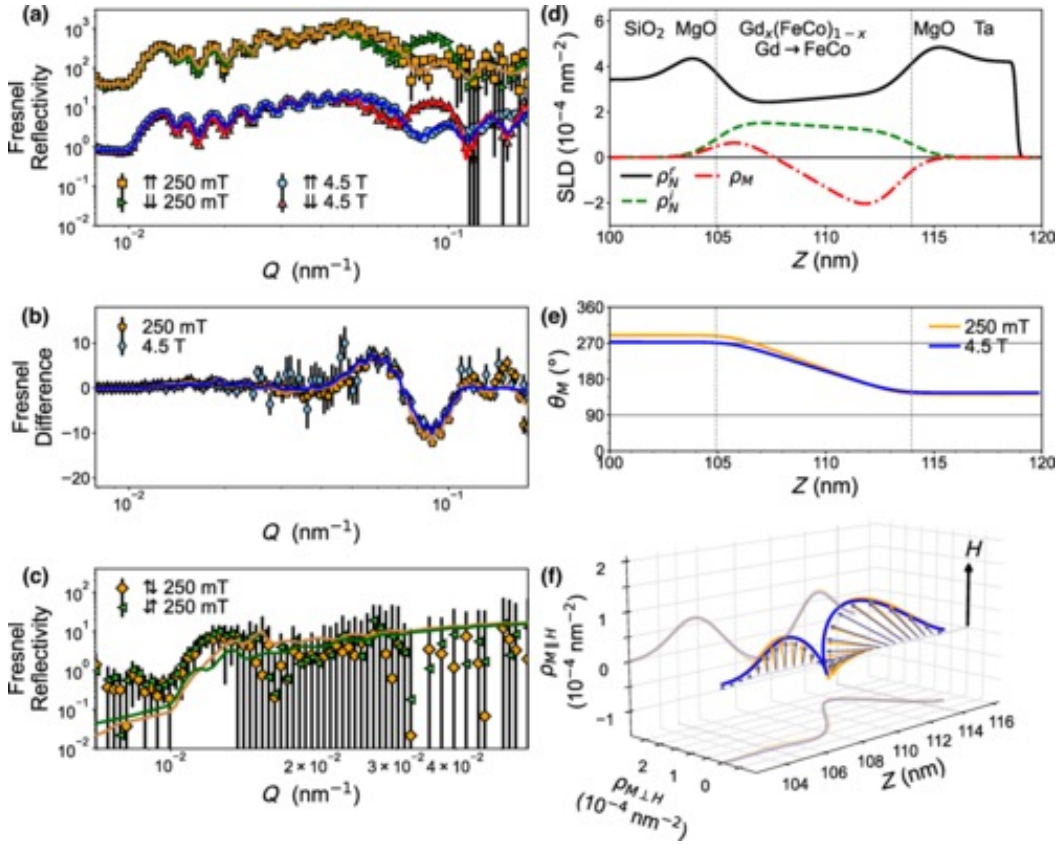
SLD's PA data plots: Not many examples in literature 3D spin structure

- Some people go for 3D plots of the magnetic structure Guo et al Phys. Rev. Applied **21**, 014045 – **2024**
- Its paramount to show multiple fields for PA data, which they do in the SI. This is because the orientation fo the sampel can really matter.
- So PA measurements need multiple orientations of the sample to be measured.



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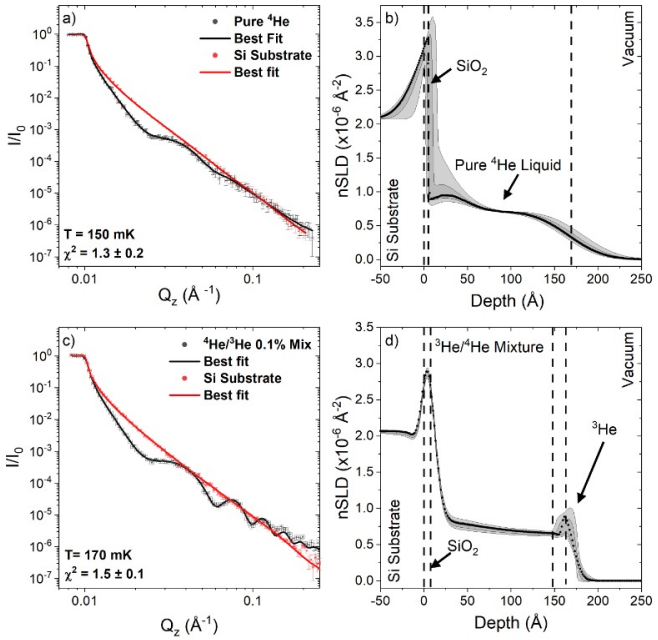
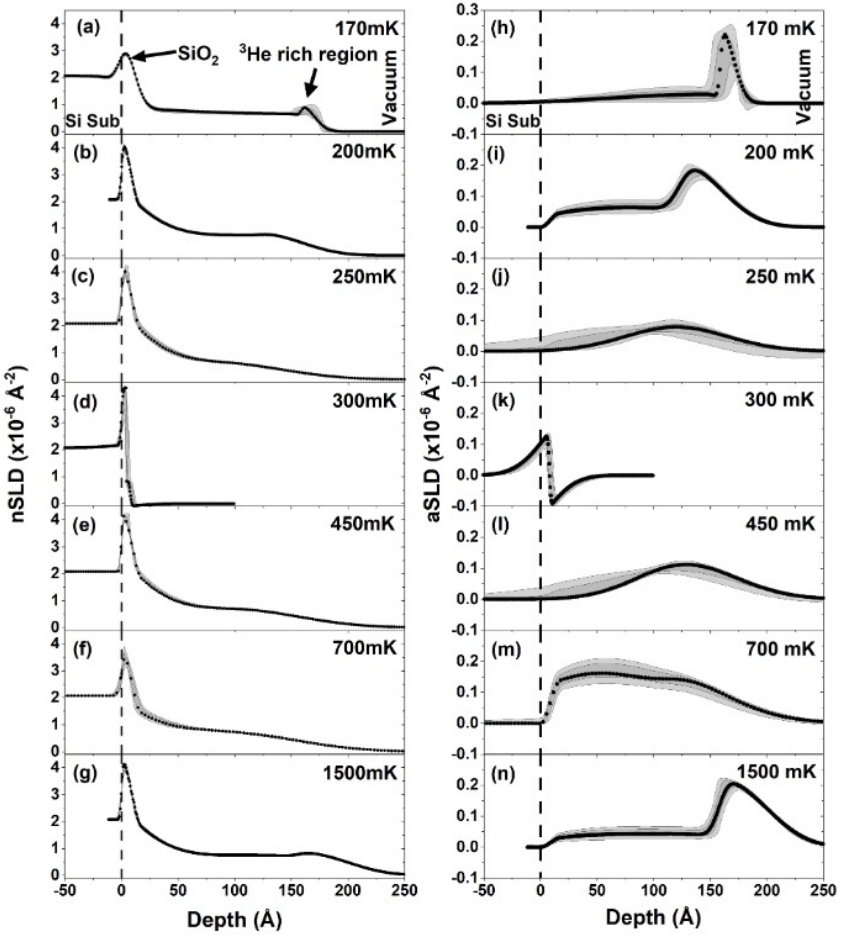
What else should we be doing are we missing?

SLD's absorption cross sections (imaginary components)

- *From Kirichek et al on He4/He3 work*
- How best do we do this?
- Really need 95% confidence intervals





Other Examples we have are on YIG with Gd

What else should we be doing/are we missing?

Distributions: This is relatively new stuff but is really really important

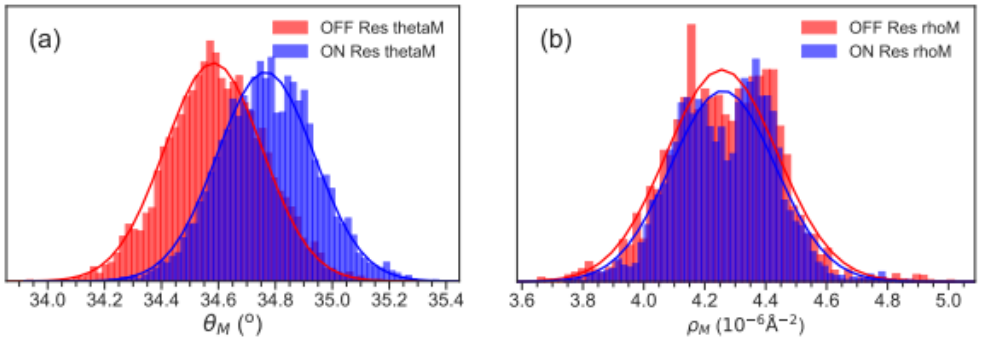
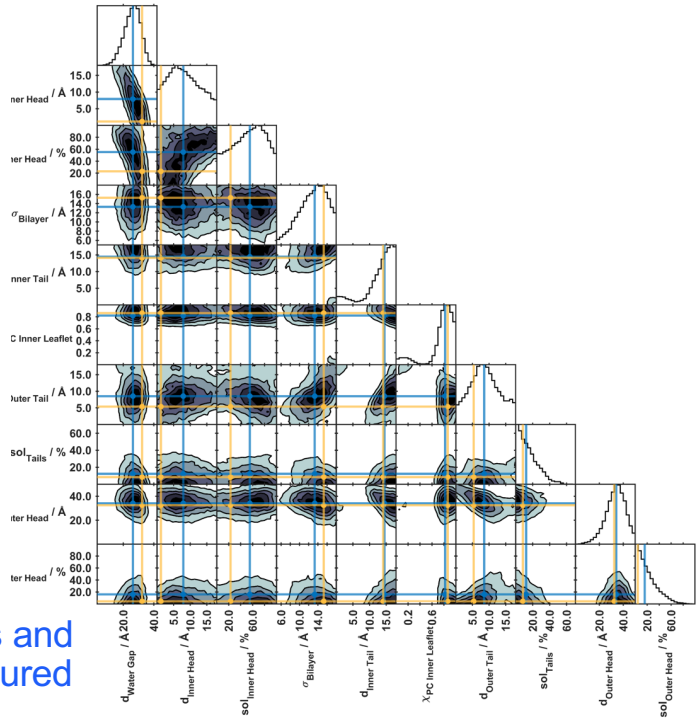


Figure 7: Probability histograms for the magnitude of the magnetisation angle (θ_M) (a) and the magnetic moment (ρ_M) (b) for the on and off states obtained from the fits shown in figure 6. The solid lines show a Gaussian fit to the histogram.



- LHS Taken from the thesis of Dan Roe another PA example loimportant,mall changes in magnetic angle and moment.
- RHS Taken from the work of Hall et al showing mixture of correlations and distributions with medium and mean/best fits marked as different coloured lines.
- **The distributions are really important, and we should be showing best fit, mean and medium positions on them maybe at a minimum and they show what your distribution of your answer actually is?**

We need to really discuss what we should show with these?

Ideally show them all or just the important parameters?

Correlation plots

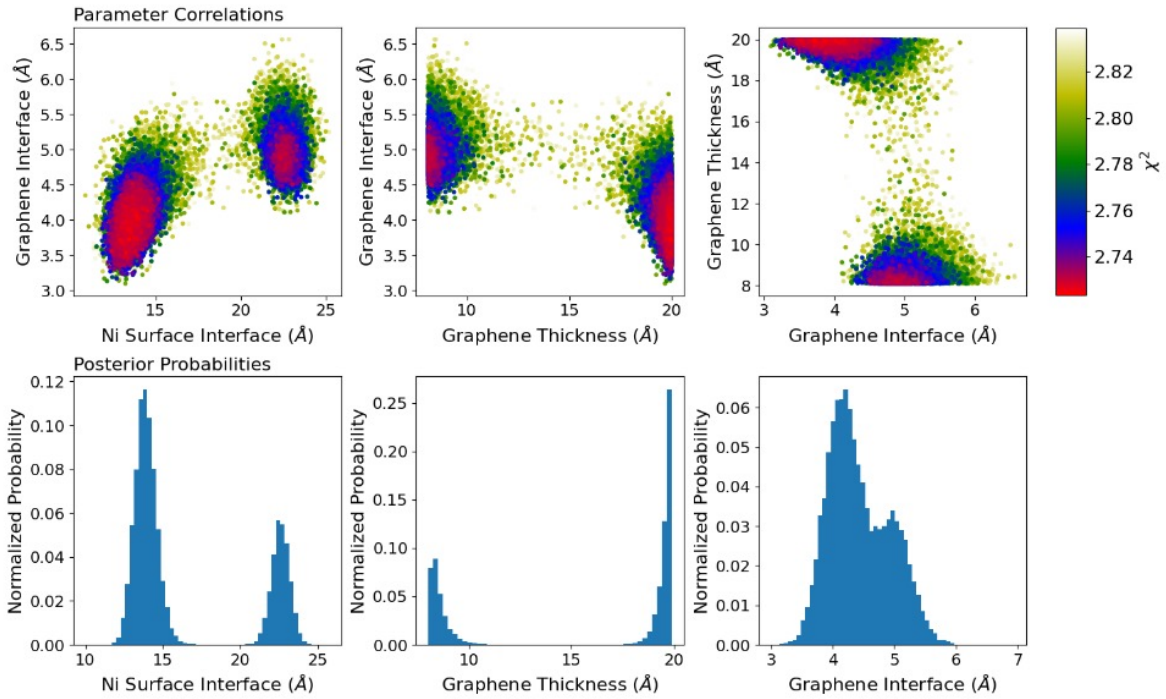


FIG. S13. Correlation plots and posterior probability distributions for the parameters exhibiting bi-modal behaviour from Model 9. Secondary information (obtained from the SEM and Raman spectroscopy measurements) was used to select one mode as preferable in each case.

- Perhaps less important but still quite important for combining secondary techniques.
- This is a graphene example allowing Raman measurements to be used to restrict priors.
- Showing full corner plots can be too difficult if you have lots of parpameters?

How should these be handled?

How important are they?

Model selection/fitting method:

- Sometimes its hard to select models especially in HCM where you have no contrasts to collapse phase space.
- We have new tools like nested samplers for the Bayesian evidence and bayes factors? How do we display them?
- Even Chi^2 plots can help.

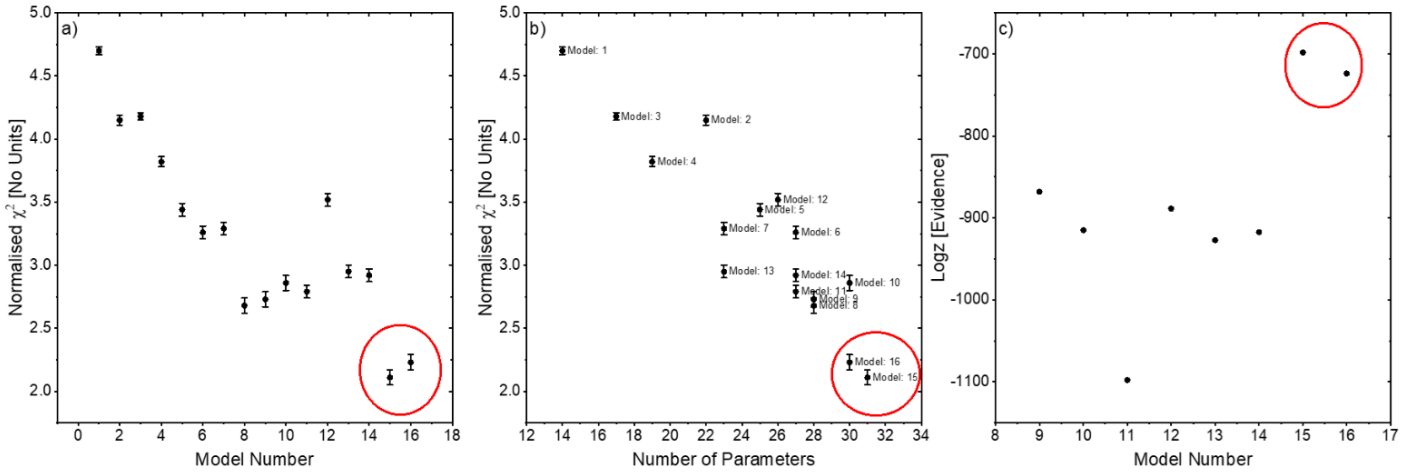


FIG. S20. Panels (a) and (b) show the trends in χ^2 vs the model number and number of parameters, respectively. Models 15 and 16 have the lowest (best) χ^2 values. However, Model 15 is dismissed as the roughness of the graphene was allowed to be non conformal to the Ni as previously reasoned to be non-physical. (c) Bayesian evidence term as computed by the UltraNest nested sampler package.[38] The least negative values are the ones that are most probable, in this case Models 15 and 16. The error bars in panel (c) are smaller than the data points.

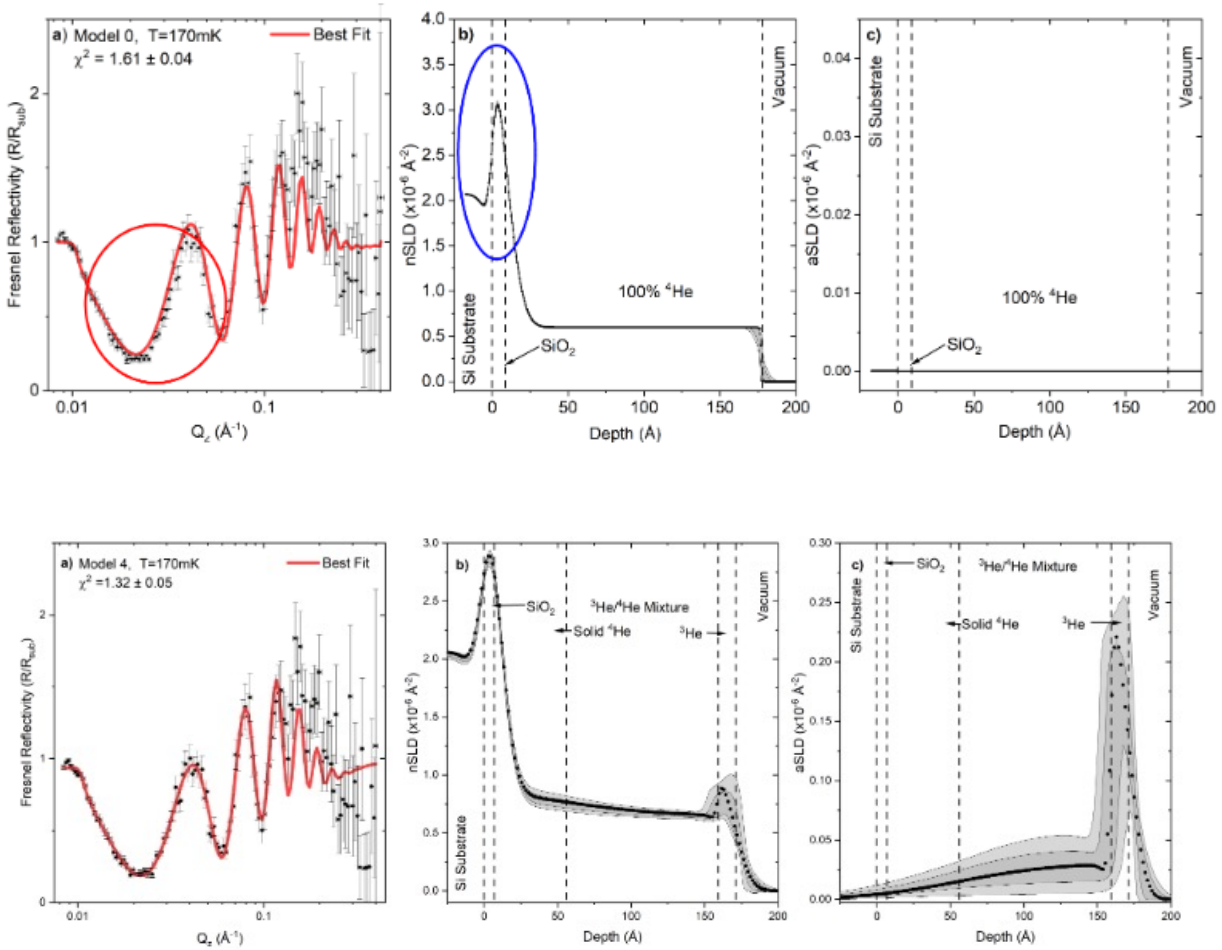
New stuff how do we utilise these if needed?

Other things to show Helium paper again:

- Model 0 or zeroth order model to show the ideal case doesn't work.
- Substrate characterisations – especially if used to constrain other models, arguable part of the fit but not shown.
- Fitting methodology for helium paper shown in SI with model 0 out to model 4 showing how model was built up?
- Questions for fitting established

In this case, the questions are:

1. Can we measure a condensed liquid helium surface and layer on the Si block?
2. Can the model confirm the presence of dilute ^{3}He in the liquid ^{4}He both for nominally pure ^{4}He and for the 0.1%^{3}He-^{4}He mixture?
3. Can we determine the distribution of the ^{3}He as a function of temperature both for nominally pure ^{4}He and for the 0.1%^{3}He-^{4}He mixture?

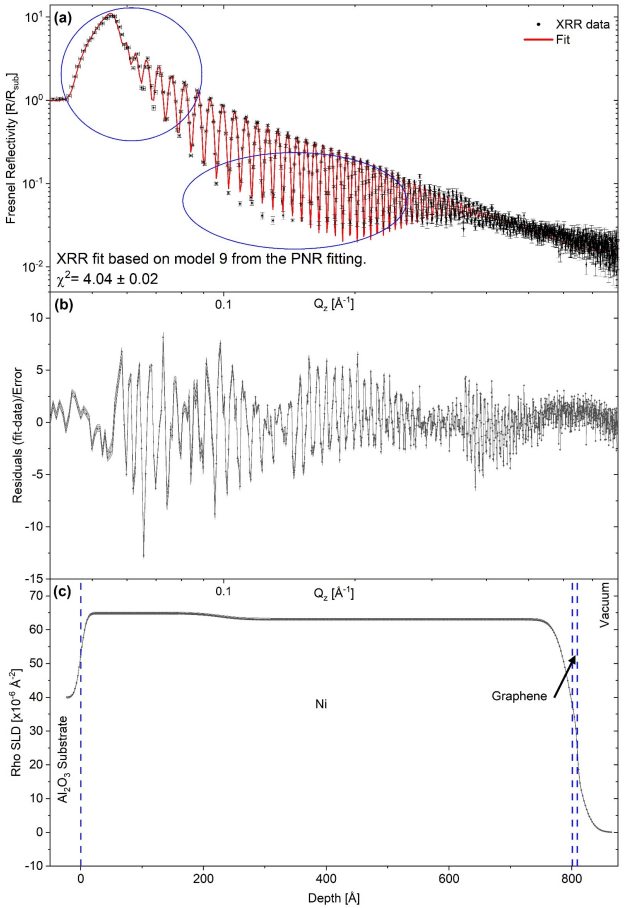


Supplementary Figure 8: Model 4: 170mK Solid thin layer of ^{4}He /^{3}He^{4}He mixture layer/thin ^{3}He layer/Vacuum. Panel a) shows Fresnel reflectivity. Panel b) shows Neutron Scattering Length density (nSLD) profile. Panel c) shows Neutron absorption profile (aSLD).

What other information to quote on how the model was fitted?

- What other information to quote on how the model was fitted?
  - Fitting Software used
  - Figure of Merrit used? Chi^2 what are you using etc if not chi^2 figure of merrit please justify and define it?
  - Minimiser? MCMC, nested sampler, etc
  - Residual plots? **Help show where fitting isn't working like critical edges**
  - **What is the analysis meant to achieve? What questions will it answer?**
  - **Offspecualr data is a whole other seminar I suspect.**

  - **What should be included?**



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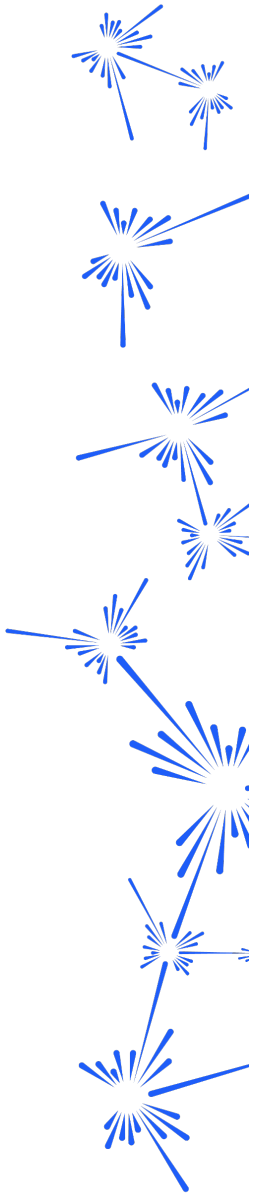
Thanks for listening



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