

Dear Editor,

We thank you for considering our manuscript titled “Neutron adiabaticity and its impact on data analysis, illustrated for polarized GISANS” of the ECNS proceedings on the poster presentation with #290.

Following the referees’ comments, we have revised the article accordingly. Point-by-point responses to every comment are given below.

According to referee #1:

Comment #1:

The paper is covering the important topic of adiabaticity for actual experiments well and addresses the possibility of using simulations of the magnetic field as well as MC ray-tracing in order to improve analysis of the scattering. An interesting example related to DWBA analysis of GISANS measurements is used as motivating case.

A general remark is that the paper should be checked for language inconsistencies. With the help of a native speaker, better clarity and overall quality could be achieved. Below are listed some problematic sentences and some improvement suggestions.

After correction taking those comments into account this paper is recommended for publication.

Reply: We thank the referee for spotting these mistakes and we have rewritten parts of the manuscript to improve the clarity. For the specific sentences raised:

1. "Significance for" instead of "significance on" (abstract line 1)

→ We use “significance of” now. To make our statement clearer, this sentence is changed to “The significance of the neutron spin adiabaticity in the data analysis of polarized Grazing Incidence Small Angle Neutron Scattering (GISANS) is discussed”

2. "Significantly impact the data analysis" instead of "impact on" (abstract, last line. And elsewhere in text)

→ After some consideration, we have altered the sentence structure, switching primarily to the use of the verb “to affect” rather than “to impact”.

Comment #2:

Since it is the central topic of the paper, the short definition of the concept of adiabaticity would be better placed much earlier in the introduction.

Reply: To address this important point, the adiabaticity is now mentioned at the very beginning of the paper, keeping the detailed calculation at the previous position.

Comment #3:

"To deal with such cases where there is a deviation..." This sentence is vague, a deviation of what, from what?

Reply: We have changed this to “To deal with these cases of critically low adiabaticity”

Comment #4:

"In this article, we demonstrate what is required, as well as the effect," This sentence is vague. What is required in terms of what and what for. As well as the effect of what on what?

Reply: We have changed this to “In this article, we demonstrate the determination of the neutron adiabaticity and polarization by a combination of magnetic field modelling and neutron ray-tracing, and the effect of an imperfect neutron transport on the data analysis, using the example of polarized GISANS from the magnetic domains and domain walls in a thin film of FePd.”

Comment #5:

It is suggested to provide references for "techniques developed to track the Larmor precession, such as Spin-Echo SANS, or spherical polarimetry techniques using cryopad or mu-pad"

Reply: We thank the referee for this important comment, and have added examples of relevant literature.

Comment #6:

"Then we demonstrate the magnetic field simulations combined with neutron ray-tracing, and discuss the effect on the analysis." –Effect of what? Is it meant as "we demonstrate how the combination on n ray tracing and magnetic field simulations can be used for data analysis"??

Reply: To be more precise, we have changed this to “In this article, we demonstrate the determination of the neutron adiabaticity and polarization by a combination of magnetic field modelling and neutron ray-tracing, and the effect of an imperfect neutron transport on the data analysis, using the example of polarized GISANS from the magnetic domains and domain walls in a thin film of FePd. Then we demonstrate the magnetic field simulations combined with neutron ray-tracing. We discuss the effect of an imperfect neutron polarization on the analysis of the magnetic domain structure by the DWBA.”

Comment #7:

The asymmetry of the GISANS pattern for the left and right peaks is not very obvious from the color coded intensity map. Maybe a 1 dimensional cut or integral of the detector images would help. Additionally, the jet color scale is known to be one of the worst possible choice for quantitative data representation: Crameri, F., Shephard, G.E.

& Heron, P.J. The misuse of colour in science communication. Nat Commun 11, 5444 (2020). <https://doi.org/10.1038/s41467-020-19160-7>).

Reply: Indeed, the 1D cut is easier to interpret. Many thanks for pointing this out, we have added it to the article.

Comment #8:

No reason is mentioned for the 20deg rotation of the maze structure wrt the main axis. Additionally, given that the actual sample is several orders of magnitude larger than the field of view covered by the single MFM image, is this specific orientation constant over the whole sample?

Reply: We thank the referee for this important question, which is indeed a typical problem of the small scan range in MFM measurements. We make several notes here:

- ➔ Note #1: the origin of a preferred in-plane domain direction can result either from the growth process, or from the magnetic field history of the sample. If coming from the growth process, three possible reasons are listed here for FePd thin films with low PMA: (i) in fully structural disordered systems of bulk cubic FePd the easy magnetization axis is along [111], leaving an easy magnetization axis along $\langle 110 \rangle$ in disordered thin films. (ii) A preferential magnetization direction in Fe and Fe/Pd thin films according to the chamber geometry and the incident Fe flux direction during growth. (iii) A substrate misorientation. If resulting from the magnetic field history, a tilt of the applied field wrt the sample surface normal during the out-of-plane saturation (as was applied for the described measurement) could result in an in-plane preferential direction.
- ➔ Note #2: we have performed several MFM investigations of an in-plane preferential domain orientation after an out-of-plane field saturation. Unfortunately, MFM could only be studied in zero field condition, and with sample transfers for every field saturation process. This complicates a comparison between different field histories on FePd with a maze domain structure. For samples with lower PMA and larger in-plane magnetization, we found that the field direction during the saturation and following demagnetization process governs the domain direction [Ye, Jianwei, "Determination of the Domain Structure of FePd Thin Films and Its Relation to the Magneto-Resistance Effects", 2020 (December), Master Thesis, RWTH Aachen]. This leads to the assumption, that also in samples with higher PMA the applied field orientation impacts strongly the domain distribution.
- ➔ Note #3: Reasons for the preferential in-plane domain orientation are discussed elsewhere and are not part of this article.

Comment #9:

In fig 6, 7, 8 it would be helpful to display the xyz coordinate system (esp. since fig 3 is shown with the electromagnet in the horizontal direction.)

Reply: We have added the coordinate systems in these figures and generally adapted some of the images.

According to referee #2:

Comment #1:

In their manuscript “Neutron adiabaticity and its impact on data analysis, illustrated for polarised GISANS” the authors describe micro magnetic simulations combined with ray tracing simulations to determine the beam de-polarization during a GI-VSANS experiment and discuss the implications on the determination of accurate magnetic scattering cross sections. The analysis of polarised grazing incidence scattering data is certainly interesting and challenging.

With the current manuscript I see one major challenge:

The need for precise knowledge of instrument polarisation performance is well known and usually taken into account by measuring the polarisation without a sample and then include this in the data analysis. On the other hand micro magnetic simulations and ray tracing simulations are done when designing instruments. I wonder how the results presented here contribute to a deeper understanding in this context as a challenging scattering geometry (GISANS) is combined with a complicated sample showing chirality. As benchmark a simple system run in standard mode on a well known Beamline might have been preferable.

Reply: The referee addresses the fundamental concept of this paper and highlights very significant points. We appreciate this and would like to comment following:

- Note #1: We agree that as a benchmark for showing the importance of a combination of magnetic simulations, ray tracing, and data analysis, a simple system would have been preferable if that as well can show the necessity of such a combination. However, especially magnetic systems with chiral structures need to be investigated with polarization analysis and a precise knowledge of the polarization vector. As an example, the DWBA analysis is more straightforward for “simpler” magnetization patterns (e.g., aligned domains), which we have as well investigated in a recent beamtime using GISANS with polarization analysis. Such systems however do not show the same non-zero chirality leading to a GISANS peak asymmetry, which in turn is very sensitive to the tilt of the polarization vector. Hence such a system is not sensitive to a tiny misalignment of the neutron polarization direction as sketched for the example in this paper.
- Note #2: Direct beam measurements without sample have been performed and showed acceptable flipping ratios around 45 (we have added this information in the article). The incident neutron polarization with $P_{in} = 0.97$ and ^3He -cell polarization of $P_{^3\text{He}} = 0.988$ together yield $P_{total} = 0.958$, which can be in

accordance with a small tilt of the neutron polarization at the sample position (especially in the shown configuration and with small guide fields of $B = 2\text{mT}$). The neutron spin rotates adiabatically after the sample into the analyzer region. We argue that small deviations of \vec{P} cannot always be pre-determined by flipping ratio measurements, but still impact the data analysis (e.g., for systems under guide field conditions, and with complex magnetic arrangements). Then, only two options can help for a detailed data analysis: (i) showing reproducibility, or (ii) the combination with magnetic modelling and neutron ray tracing as performed in this paper. The reproducibility of measurements is always an important point which we have addressed also by performing these measurements again recently, and which yield similar results with a measurable net-chirality despite high flipping ratios. This shows again that tiny deviations of \vec{P} with respect to the intended direction impact much more the data analysis than believed. The shown combination of magnetic modelling and ray tracing may therefore help not only to guide the preparation of following beamtimes and to improve the beamline setup, but also help in understanding what all can impact the measured data and what needs to be considered for reproducibility and data publication.

Comment #2:

Is equation 1 defined in this paper or is there a reference for it?

Reply: It is defined here. To make this clearer, we have rewritten it to “The adiabaticity is defined by the ratio of the Larmor frequency of the neutron spin ω_L ”

Comment #3:

Cryopad and mupad may need references as well. What is Spin-Echo SANS?

Reply: We have added references accordingly.

Comment #4:

Page 1: The statement that uniaxial polarisation analysis does not measure components of the polarisation perpendicular to the field seems confusing. Spin flip measures the magnetisation perpendicular to the polarization

Reply: Yes, both are correct. The uniaxial polarization analysis only measures the neutron polarization component parallel to B (unlike e.g. spherical polarimetry as stated in the text). By measuring the change in that polarization component, it measures the sample magnetization perpendicular to neutron polarization, as the magnetization would affect the polarization in the form of spin-flip scattering as the reviewer has indicated. We've made the text more concise by using “neutron polarization” instead of “polarization”, e.g. page 1, paragraph 3: “Our experiment

belongs to a class of polarized neutron experiments known as uniaxial polarization analysis [1], which measures the component of neutron polarization along \vec{B} .”

Comment #5:

It may be worth mentioning that neutrons are only sensitive to moments perpendicular to Q.

Reply: This statement has been added after introducing \vec{M}_\perp in Eq. (5): “ \vec{M}_\perp is Fourier transform of the sample magnetization perpendicular to the scattering vector \vec{Q} , with its complex conjugate \vec{M}_\perp^* , and I_{Si} the nuclear spin-incoherent scattering intensity. This shows that only magnetization components perpendicular to \vec{Q} are measured.”

Comment #6:

The definition of Q in equation is very confusing. Usually, Q denotes the momentum transfer, as also done later in the manuscript.

Reply: Q is a common definition for the quality factor (strength of the magnetocrystalline anisotropy in ferromagnetic thin films), but indeed confusing here. We have changed it to $K=K_u/K_{sh}$.

Comment #7:

There are a couple of unusual expressions, e.g. the sample in question..., formed in between..., MFM measurement (image?), high domain width, two be able to lead to... I propose the native speakers among the authors double check the language.

Reply: We thank the reviewer for pointing this out and have rewritten some of the sentences accordingly.

Comment #8:

Caption Fig. 1: Why define c separate from the coordinate system. At least, say that c is along y or -y.

Reply: Due to the maze domain structure, c can be along x or y here. I have changed the text to: “The sketch in Fig. 1(b) assumes chiral Bloch walls with a preferred orientation of chirality \vec{C} parallel to the thin film surface (i.e., in the x-y-plane)”

Comment #9:

Equation 3 is an approximation, as both the sin and cos are Taylor expanded. Say so.

Reply: We have rephrased this to “Using the small-angle approximation, the scattering vector Q is described by...”

Comment #10:

Fig. 2: I wonder where the horizon is and if the GISANS is not at the horizon, why it is so.

Reply: Does the referee mean the plane of the sample surface with “horizon”? If yes, here only scattering from the edges of the sample is expected and not of importance for the GISANS analysis. Instead, the GISANS peaks occurring at an incidence angle of $\Theta_i = \Theta_f$ are displayed. Hence, the horizon is not displayed in I⁻ and I⁺ measurements in Figure 2(b).

Comment #11:

What is the vector or a matrix?

Reply: Does the referee mean $\vec{\sigma}$ and \vec{b}_l ? Both are vectors, where $\vec{\sigma}$ is the vector of Pauli-matrices. I have emboldened $\vec{\sigma}$ and \vec{b}_l .

Comment #12:

How do you define the main axis in Fig. 6? Main with respect to what?

Reply: Due to the thin film rectangular shape, the sample was aligned with two opposite edges parallel to the incident neutron beam, giving the “main axis here”, i.e., the x-axis, or neutron beam direction. We apologize for the unclear sentence and changed it to: “around a mean angle tilted by 20° away from the incident neutron beam direction”.

We hope that we have replied to all the comments to the reviewers' satisfaction. We are looking forward to a positive response.

Yours sincerely,



Annika Stellhorn