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Reconstruction of magnetic profiles from polarized reflectivity data

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Abstract

An iterative algorithm for the reconstruction of magnetic profiles from polarized neutron reflection data is presented. The new algorithm avoids the use of a reference layer and makes use of the frequently available knowledge on the sequence of the layers. The features of the algorithm are studied in several examples and satisfactory convergence to the true profile is found for realistic magnetic field strengths.

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Keywords: Specular reflection; Multilayers; Magnetic profiles

1. Introduction

Neutron specular reflection is a widely used tool in materials science [1]. Especially, the study of thin films and superlattices via neutron reflectometry has led to a deeper knowledge of these systems. Making use of the spin-degrees of freedom represents an essential progress in neutron reflectometry. Because of the magnetic moment and vanishing electrical charge of the neutron, this so-called spin-polarized neutron reflectometry is best suited to investigate the magnetic structure of layered specimens.

Measurements with standard reflectometer set-ups usually provide only the moduli of the reflection matrix elements, while the phases remain undetermined. A unique profile reconstruction requires, however, the knowledge of the full reflection matrix (moduli and phases) for all energies. Several solutions of this so-called *phase problem* have been suggested. Among these the reference layer methods which make use of the spin-dependent interaction of the neutron with a magnetic field are most promising [2–5]. Despite the importance of these suggestions, to our knowledge only the method of Ref. [5] has been implemented experimentally for a specific case [6] so far. One severe drawback of these methods is the fact that the use of reference layers requires manipulations of the specimen and may generate uncontrolled changes of the sample.

In this contribution we present a method for the unique reconstruction of magnetic profiles from spin-polarized reflection data. We do not use a reference layer, but we make use of the specific form of the reflection matrix in the presence of a magnetic field and assume that we have good knowledge of the layer structure from the generation of the sample and/or the analysis by X-rays or other means.

2. Iterative magnetic profile reconstruction

Neutron specular reflection is essentially quantal scattering in one dimension by a potential

$$\mathscr{V}(x) = \mathscr{V}_{\mathrm{nucl}} + \mathscr{V}_{\mathrm{magn}} = V_{\mathrm{nucl}}(x)\mathbf{1} + \gamma\boldsymbol{\sigma}\cdot\mathbf{B}(x), \tag{1}$$

which depends only on the coordinate x perpendicular to the surface. Here, $\boldsymbol{\sigma}$ is the vector formed by the Pauli matrices which is proportional to the spin of the neutron $\mathbf{s} = (\hbar/2)\boldsymbol{\sigma}$. Hence, the potential is a 2×2 matrix with the diagonal nuclear part $V_{\mathrm{nucl}} = 4\pi\rho(x)$ given by the scattering-length density profile $\rho(x)$. The magnetic contribution depends linearly on the magnetic field vector $\mathbf{B}$. The quantity $\gamma = -g_{\mathrm{s}}\mu_{\mathrm{N}}m_{\mathrm{n}}/\hbar^2$ is given by the nuclear magneton μ_{N}, the mass m_{n} of the neutron and its gyromagnetic

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spin-factor $g_s = -3.826$. Following Ref. [3] the reflection of a neutron beam is described by a 2×2 matrix $\mathscr{R}$ which can be cast into the form

$$\mathscr{R} = \begin{pmatrix} R_{++} & R_{+-} \\ R_{-+} & R_{--} \end{pmatrix} = R_{\mathrm{tr}} \mathscr{H}, \tag{2}$$

where $R_{\mathrm{tr}} = |R_{\mathrm{tr}}| \exp(\mathrm{i}\varphi_{\mathrm{tr}}) = (R_{++} + R_{--})/2$. The indices $\pm\pm$ and $\pm\mp$ refer to the spin components of the incident and reflected beam, respectively. The 2×2 matrix $\mathscr{H}$ can be determined by a set of polarization measurements of the reflected beam [3,7]. This is even true for incomplete polarization measurements as shown in Ref. [8]. Thus, the $\mathscr{R}$-matrix can be fully determined by experiment up to a common phase, e.g. φ_{tr}.

Frequently one has information about the layers of a sample from its production and/or from previous X-ray measurements. Therefore it is reasonable to consider experiments, where V_{nucl} is known and only the reconstruction of the magnetic field distribution $\mathbf{B}(x)$ is requested. In the absence of a magnetic field the knowledge of V_{nucl} allows the evaluation of the full reflection matrix $\tilde{\mathscr{R}}(x) = |R_{\mathrm{nucl}}| \mathrm{e}^{\mathrm{i}\varphi_{\mathrm{nucl}}} \mathbf{1}$. In the presence of sufficiently small magnetic fields we can apply perturbation theory and obtain for the phase of R_{tr} in first order approximation $\varphi_{\mathrm{tr}}^{(0)} = \varphi_{\mathrm{nucl}}$. On the basis of this approximation we make a first ansatz,

$$\tilde{\mathscr{R}}^{(0)} = |R_{\mathrm{tr}}| \mathrm{e}^{\mathrm{i}\varphi_{\mathrm{nucl}}} \mathscr{H}, \tag{3}$$

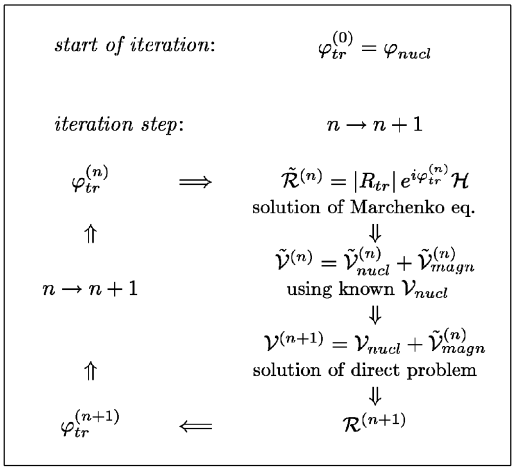

Fig. 1. Scheme of the iterative algorithm for the reconstruction of the magnetic profile. For explanation see text.

to start the iteration procedure. Solving the Marchenko equation (see e.g. Ref. [9]) for $\tilde{\mathscr{R}}^{(0)}$ we can reconstruct the corresponding potential $\tilde{\mathscr{V}}^{(0)}$ from which we separate $\tilde{V}_{\mathrm{nucl}}^{(0)}$ and $\tilde{\mathscr{V}}_{\mathrm{magn}}^{(0)}$. In the next step we solve the direct problem for the potential $\mathscr{V}^{(1)} = \mathscr{V}_{\mathrm{nucl}} + \tilde{\mathscr{V}}_{\mathrm{magn}}^{(0)}$ and obtain the new value $\varphi_{\mathrm{tr}}^{(1)}$ which in turn is used to determine a new reflection matrix $\tilde{\mathscr{R}}^{(1)}$. Repeating the procedure several times we expect convergence to the true magnetic profile. A scheme of this iterative process is shown in Fig. 1.

It should be remarked that a similar iterative method can be developed on the basis of the representation,

$$\mathscr{R} = \begin{pmatrix} R_{++} & R_{+-} \\ R_{-+} & R_{--} \end{pmatrix} = R_{\mathrm{av}} \mathscr{K}, \tag{4}$$

with $R_{\mathrm{av}} = |R_{\mathrm{av}}| \exp(\mathrm{i}\varphi_{\mathrm{av}}) = \sqrt{R_{++} R_{--}}$. The results and the convergence are quite similar to the reported methods and will not be discussed further in this contribution.

3. Example

The iterative method presented in Fig. 1 is numerically straightforward and we have applied it to several realistic examples. These calculations indicate the feasibility of the algorithm and lead to convergence of the extracted magnetic profiles for realistic magnetic field strength **B**.

In the following we show the capability of the algorithm by its application to a schematic example. Specifically, we consider specular neutron reflection from the layered structure given in Table 1. Since we are only interested in the quality of the algorithm with regard to the reconstructed magnetic profiles, we have not included non-magnetic layers (e.g. thin Cr-layers between the Fe-layers) in this schematic sample. However, this simplification should not change the final conclusions.

Using $\mathscr{R}$-matrix values extracted from reflectivity and polarization data up to $q_{\max} = 1.5\,\mathrm{nm}^{-1}$, we applied the iterative algorithm and obtained the magnetic fields displayed in Fig. 2. The results clearly indicate the fast convergence of the algorithm towards the true magnetic field distribution. The layer structure and the different directions of the **B**-field are well reproduced. The deviations at large x-values are not a specific weakness of the present algorithm, but a direct consequence of the ill-posedness of inverse problems. These instabilities restrict the resolution in depth of any reconstruction algorithm and

Table 1
Layer structure and parameters of the schematic example

Layer number	Material	Depth (nm)	V_{nucl} (nm^{-2})	B_x (T)	B_y (T)	B_z (T)
1	Fe	0 – 8	0.010065	1.647	0.951	−1.098
2	Fe	8 – 16	0.010065	−0.776	0.776	1.902
3	Ni	16 – 24	0.011818	−0.115	−0.431	−0.446
4	Si	24 – ∞	0.002605	–	–	–

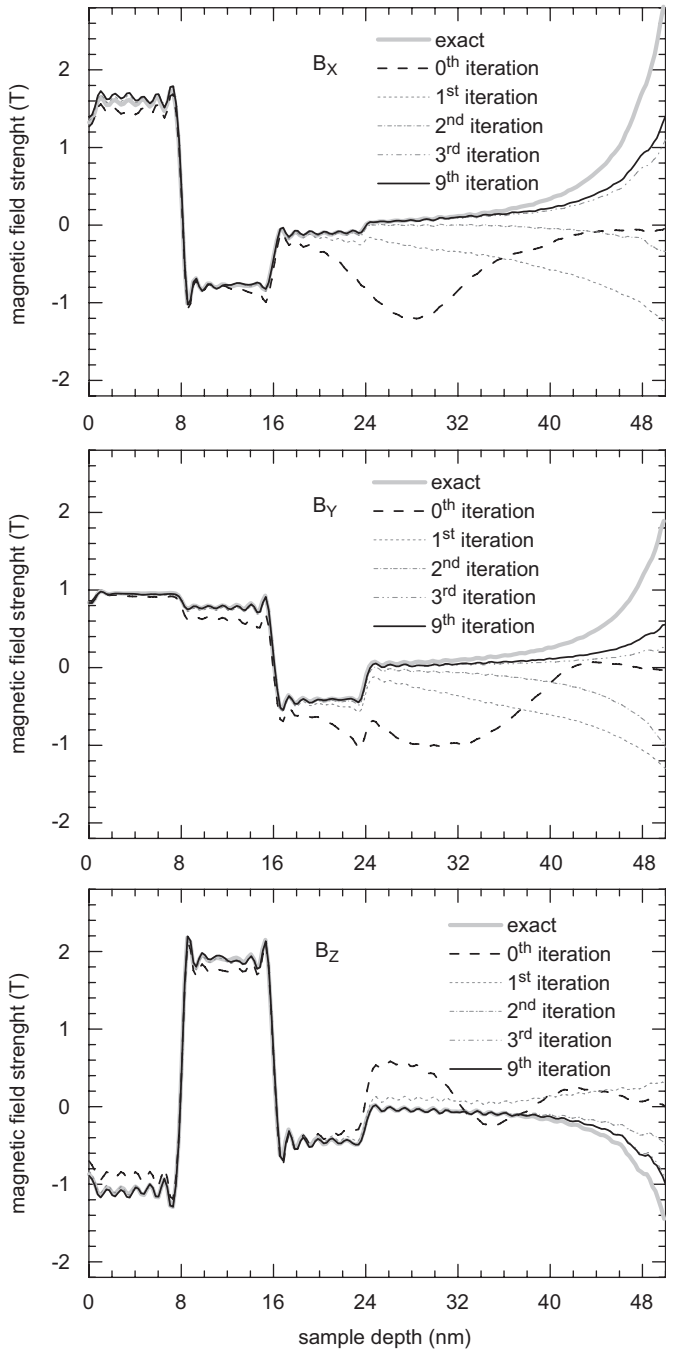

Fig. 2. Reconstruction of magnetic fields and layers of the schematic example of Table 1 by the iterative procedure.

can only be avoided via systematic inclusion of additional a- priori information.

We achieved similar reproductive power for almost all considered examples. Only for strong magnetic fields ($B \geqslant 3$ T) failures of convergence were observed for specific cases.

4. Conclusions

We presented and successfully applied an iterative procedure to reconstruct the internal magnetic fields from spin-polarized neutron reflectivity data. The method is very promising because it does not require a reference layer and it seems to converge to a unique profile. The assumption on the knowledge of the layer structure will be satisfied in many practical applications either from the production of the sample or by additional experiments, e.g. with X-rays. In addition, the iterative algorithm is very flexible and also allows the inclusion of more complex a- priori knowledge in order to improve the depth of reconstruction. Work in this direction is in progress.

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