

Detection of Multilayer Nano Structures by One Directional Polarization Analysis in Neutron Reflectometry

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Abstract: Due to the sensibility of neutron spin to the intrinsic magnetic field of magnetic materials, polarized neutron reflectometry is widely used in investigation of magnetic properties of nano-structures. Type and thickness of a multilayer can precisely be determined by measuring the polarization of reflected neutrons from the sample. In the past decades, several theoretical methods have been worked out to determine the type and thickness of thin films as a function of scattering length density (SLD) of the sample based on polarization analysis. However, as the technology of available reflectometers is limited in a way that the polarization of the reflected neutrons can be measured in the same direction as the polarization of the incident neutrons, these methods have to be modified by considering this limitation. In this paper, we have proposed a method for determining the SLD of a multilayer based on using a magnetic substrate and polarization measurement of reflected neutrons in the same direction as the polarization of incident beam. Our method, resolves this problem for available neutron reflectometers.

Key words: Polarized neutron reflectometry • Phase problems • Polarization analysis • Nano thin films • scattering length density • Magnetic substrate

INTRODUCTION

Measuring the intensity of reflected neutrons from a multilayer thin film would not solely lead to a unique result for the depth profile of the films as a function of scattering length density of the sample. In order to obtain a unique result for the SLD of the sample, the knowledge of the phase and amplitude of complex reflection coefficient, $r(q)$, as a function of neutron wave vector q , is required [1, 2]. In the past decades, several methods have been worked out to determine the phase of reflection such as reference layer [3, 4, 7] and variation of surrounding medium [5-6] which are based on the interference between the reflections of a known reference layer and an unknown part.

Recently, several new approaches in determining the phase of reflection have been proposed which are based on the measurement of polarization of reflected neutrons from magnetic multilayers such as the one which is developed by Leeb *et al.* [8-9] or those ones which are worked out with us [10-12]. These methods are based on

several measurement of polarization of reflected neutrons in different directions. However, in spite of their rich theoretical backgrounds, these methods can not be experimentally implemented because available reflectometers are limited in the measurement direction of neutron polarization in a way that the polarization of the reflected neutrons can only be measured in the same direction as the polarization of the incident beam [11-12]. In this paper, we have proposed a method which is based on the polarization analysis of the reflected neutrons in the same direction as the polarization of the incident beam. The method is capable of experimental implementations and contains more simple formulation in compared with hitherto reported works.

MATERIALS AND METHOD

Consider an unknown layer which is mounted on top of a magnetic substrate, (Figure 1). The SLD of the magnetic substrate is proportional to $(\rho(x) \pm \rho_m)$ where, $\rho_m = \frac{m}{2\pi\hbar^2} \mu_B$, is the magnetic SLD of the sample, ρ is

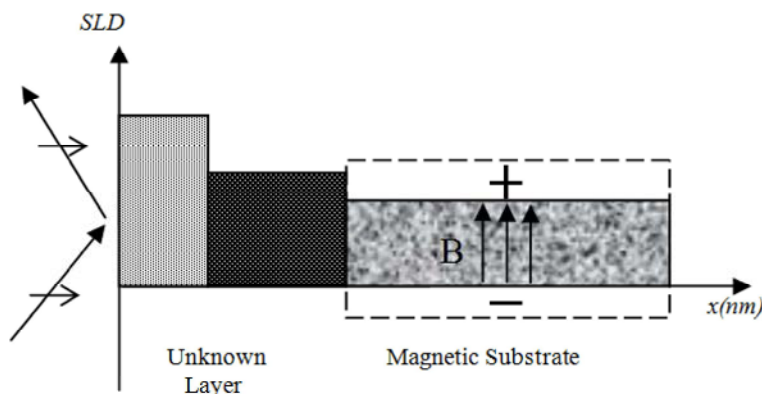


Fig. 1: Arrangement of a sample for investigating the method. Dashed line represents the effective potential experienced by neutrons due to the presence of magnetic field, B, inside the substrate.

the SLD at depth x from the surface, B is the magnetic field and μ is magnetic moment of neutrons. The two signs for the second term refer to neutrons polarized parallel and anti-parallel to the local magnetization, respectively [1, 2]. Reflection (r_{\pm}) and transmission (t_{\pm}) coefficients of the sample are determined by using the transfer matrix method [1, 2]:

$$\begin{pmatrix} 1 \\ ih_{\pm} \end{pmatrix} t_{\pm} e^{iqL} = \begin{pmatrix} A(q) & B(q) \\ C(q) & D(q) \end{pmatrix} \begin{pmatrix} 1 + r_{\pm} \\ if(1 - r_{\pm}) \end{pmatrix} \quad (1)$$

The elements of the transfer matrix, A , B , C and D , are uniquely determined by the SLD of the sample. And h_{\pm} is the refractive index of the magnetic substrate [2]:

$$h_{\pm}(q) = \left(1 - \frac{4\pi(\rho \pm \rho_m)}{q^2}\right)^{1/2}, \quad r_{\pm}(q) = \frac{\beta_{\pm}^{fh} - \alpha_{\pm}^{fh} - 2i\gamma_{\pm}^{fh}}{\beta_{\pm}^{fh} + \alpha_{\pm}^{fh} + 2} \quad (2)$$

Using equation (1) reflectivity, $R_{\pm}(q) = |r_{\pm}(q)|^2$, can be written in terms of new defined quantities, Σ_{\pm} , as follows [2, 10]:

$$\Sigma_{\pm} = fh_{\pm}^{-1}\tilde{\alpha}_{\pm}^{ff} + h_{\pm}f^{-1}\tilde{\beta}_{\pm}^{ff} = h_{\pm}(A^2 + B^2) + (h_{\pm})^{-1}(C^2 + D^2) \quad (3)$$

where

$$\begin{aligned} \alpha_{\pm}^{fh} &= h_{\pm}f^{-1}A^2 + (fh_{\pm})^{-1}C^2, & \beta_{\pm}^{fh} &= fh_{\pm}B^2 + fh_{\pm}^{-1}D^2 \\ \gamma_{\pm}^{fh} &= h_{\pm}AB + h_{\pm}^{-1}CD \end{aligned} \quad (4)$$

The tilde denotes the mirror-reversed unknown film and the superscript ff represents the same surrounding on both sides which in our case is vacuum.

The polarization of incident (p_x^0, p_y^0, p_z^0) and reflected (p_x, p_y, p_z) neutrons, are related to the reflectivity of the sample as follows [8] and [11-12]:

$$\frac{p_x p_x^0 + p_y p_y^0}{p_x^2 + p_y^2} = 1 + 2 \frac{2 - (\frac{h_+}{h_-} + \frac{h_-}{h_+}) - p_z^0(\Sigma_+ - \Sigma_-)}{\Sigma_+ \Sigma_- + 2p_z^0(\Sigma_+ - \Sigma_-) - 4} \quad (5)$$

$$p_z = \frac{2(\Sigma_+ - \Sigma_-) + p_z^0(\Sigma_+ \Sigma_- - 4)}{(\Sigma_+ \Sigma_- - 4) + 2p_z^0(\Sigma_+ - \Sigma_-)} \quad (6)$$

Suppose the incident beam to be fully polarized in x or y direction and using Eq. (3), Eq. (5) can be written as follows:

$$(h_+ h_-)^2 (A^2 + B^2)^2 + (C^2 + D^2)^2 + 2h^2 (A^2 + B^2)(C^2 + D^2) = \zeta \quad (7)$$

where

$$\zeta = 4h_+ h_- + 2(h_+ - h_-)^2 / (1 - P) \quad (8)$$

is a known parameter. P is the polarization of reflected beam in the same direction as polarization of the incident beam which is a measurable parameter in available reflectometers. h is the refractive index of the substrate for non-polarized incident beam and $h^2 = (1 - 4\pi\rho/q^2)$. Eq. (7) is the basic relation in our method which enables us to determine two unknown parameters ($A^2 + B^2$) and ($C^2 + D^2$). If P is measured for two different nonzero magnetic fields in the magnetic substrate, we can find ($A^2 + B^2$) from Eq. (7) as follows:

$$(A^2 + B^2) = \pm \sqrt{\frac{\zeta_1 - \zeta_2}{(h_1 + h_{1-})^2 - (h_2 + h_{2-})^2}} \quad (9)$$

where h_{is} , ($i=1,2$), is the refractive index of the substrate for the two different applied magnetic fields (B_1, B_2). Alternatively, Eq. (9) can directly be written in term of the magnetic fields:

$$(A^2 + B^2) = \pm \left(\frac{q^2 \hbar^2}{2\mu m} \right) \sqrt{\frac{\zeta_1 - \zeta_2}{B_2^2 - B_1^2}} \quad (10)$$

Equation (10) is the substantial equation of our method which has not reported hitherto. This equation simplifies our recent published paper [11-12] since instead of many known parameters which depend on known layer, we must only two parameters h_+ and h_- .

Using Eq. (7) and (10), the term $(C^2 + D^2)$ can readily be deduced. These two parameters determine the reflection coefficient of the free reversed unknown layer as follows:

$$\tilde{r}(q) = \frac{(A^2 + B^2) - (C^2 + D^2) \pm 2i\sqrt{(A^2 + B^2)(C^2 + D^2)} - 1}{(A^2 + B^2) + (C^2 + D^2) + 2} \quad (11)$$

From Eq. (11), we can infer that: knowing $(A^2 + B^2)$ and $(C^2 + D^2)$ would lead to two different possibilities. However, as it will be shown in the following example, only one of the results is physically acceptable. The physical solution is readily identified in most cases based on this fact that as $q \rightarrow 0$, $r(q) \rightarrow -1$ through negative values (predominantly positive SLD) or positive values (predominantly negative SLD) [6].

Numerical Example: In order to test the method numerically, we consider a bilayer (as unknown film) composed of 20 nm thick Ni over a 30 nm thick Pt with the SLD of 9.4 and $6.34 \times 10^{-4} \text{ nm}^{-2}$ for Ni and Pt respectively. As shown in Fig. 1, it is supposed the sample is mounted on top of a Co substrate with the SLD of $2.26 \times 10^{-4} \text{ nm}^{-2}$ for non-magnetized state and the incident neutrons are fully polarized in the x direction. In order to determine the term $(A^2 + B^2)$ from Eq. (10), we have to use two different substrate. Practically, mounting the main sample over two different substrates and obtaining the same structure for the sample is not possible (Experimental process of sample preparation would not lead to obtaining exactly the same sample but with different substrate). In order to resolve this problem, we can use a magnetic substrate with two different quantization orientations which are obtained by applying two different magnetic fields with different magnitudes (B_1, B_2) to the substrate. To prevent from obtaining negative values for the term $(\zeta_1 - \zeta_2)/(B_2^2 - B_1^2)$ which would hamper the numerical calculations, we propose the second field, B_2 , to be stronger than B_1 .

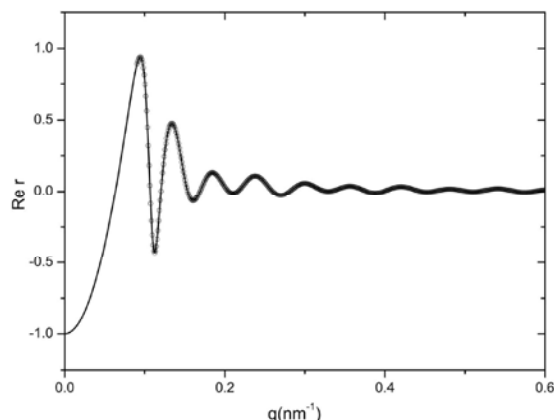


Fig. 2: Solid line: $\text{Re } r(Q)$ for the mirror image of the film without backing of Fig. 1. Circles: $\text{Re } r(Q)$ as recovered from the two measurement of ζ for two different magnetic field for larger values than critical Q of the substrate.

We consider two magnetic field which one of them, (B_2), magnetize the substrate to its saturated state with magnetic scattering length density of $\pm 4.12 \times 10^{-4} \text{ nm}^{-2}$ and the other, (B_1), leads to magnetic SLD of $\pm 2.91 \times 10^{-4} \text{ nm}^{-2}$ for the substrate. Plus (minus) sign denotes the direction parallel (anti parallel) to the direction of spin quantization in the magnetic substrate.

Fig.2, illustrates the real part of reflection coefficient, $\text{Re } r(q)$, for mirror reversed image of the sample of Fig. 1 without backing. Using Eq. (10) for the two orientations of magnetic fields and measuring the polarization of reflected neutrons in the same direction as the polarization of the incident neutrons for each field, the term $(A^2 + B^2)$ is readily determined. By knowing $(A^2 + B^2)$, the other term, $(C^2 + D^2)$, is deduced from the knowledge of ζ parameters for each of the magnetic field orientations from Eq. (7).

The circled curve in Fig.2, represents the data of $\text{Re } r(q)$ for larger values than critical q of the substrate. The data below the critical q can readily be interpolated from the fact that $r(q) \rightarrow -1$ as $q \rightarrow 0$ [6].

The imaginary part of the reflection coefficient for the mirror image of the sample without backing, $\text{Im } r(q)$, is also determined by knowing $(A^2 + B^2)$ and $(C^2 + D^2)$ from Eq. (11). Since Eq. (11) would lead to two different solution for the imaginary part of the reflection coefficient, the physical solution is chosen based on this fact that as $q \rightarrow 0$, $r(q) \rightarrow -1$ through negative values (predominantly positive SLD) or positive values (predominantly negative SLD). As it is shown in Fig.3, the circles and squares show the two different solution for $\text{Im } r(q)$. The physical branch alternates between these sets.

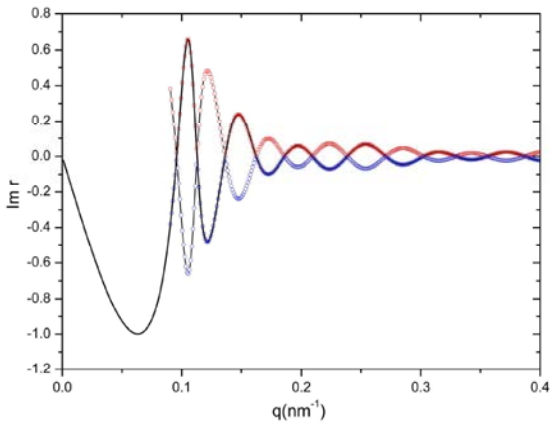


Fig. 3: Solid line: $\text{Im}r(Q)$ for the mirror image of the film without backing of Fig. 1. Circles (blue) and squares (red): the two possible values of $\text{Im}r(Q)$ obtained from the recovered $\text{Re}r(Q)$ and $R(Q)$, as described in the text. The physical branch alternates between these sets.

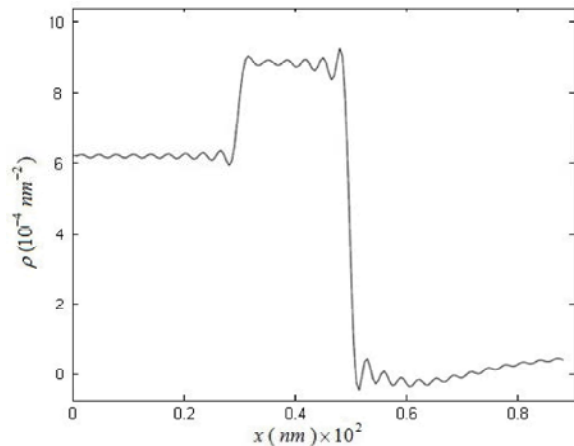


Fig. 4: The retrieved SLD for the mirror image of the sample of Fig.1 without backing using the Sacks Code [13-14].

Figure 4, demonstrates the retrieved SLD for the mirror image of the sample of Fig. 1 without backing. Once $r(q)$ is determined in the whole range of the q values, the SLD of the sample can be retrieved using the Gel'fand-Levitan-Marchenko integral equation [2]. In order to retrieve the scattering length density of the sample, we use the real and imaginary parts of the reflection coefficient as input in some certain codes such as the one which is developed by P. Sacks [13-14]. As it is illustrated in the figure, the retrieved SLD for the mirror image of the sample of Fig.1 without backing is clear.

CONCLUSIONS

We have proposed a method to determine the modules and phase of reflection coefficient by using a magnetic substrate and polarization measurement. The method takes into account the limitation of available reflectometers in polarization analysis in which the polarization measurements of reflected beam can only be performed in the same direction as the incident beam. In comparison with other methods which make use of polarization measurements such as those which are worked out by Leeb [8-9] and us [11-12], this new approach requires just two measurement of polarization in the same direction for two different external magnetic field. No reflectivity data is required and the relations are simpler and more straightforward which reduce the practical complexities of the method. Finally, a unique profile for the SLD of the multilayer is retrieved which determines the type and thickness of the layers. The method seems experimentally feasible for thin films over a magnetic substrate and we look forward to its experimental implementation.

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