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Exact determination of phase information in spin-polarized neutron specular reflectometry

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Abstract. A method is proposed to determine the complex reflection coefficient of any real scattering length density (i.e., in the case where there is no effective absorption, which is a good approximation for neutrons) in neutron specular reflectometry. The method makes use of a magnetic reference layer mediated between the substrate and an unknown sample and measurements of the polarization direction of the reflected beam or a suitable choice of polarization and reflectivity analysis of the reflected beam. It corresponds to the concept proposed recently, but has been derived in the formalism of the transfer matrix. The method is based upon relations between the polarization of the incident and reflected beams, and the transfer matrix elements of the unknown and known layers. Thus, in this manner, only by final polarization orientation measurement can we find the reflection coefficient of any unknown sample which is surrounded on both sides by a uniform medium. Apart from the final polarization orientation measurement of the reflected beam, which is hampered by complications in selecting the physical solution, we show that the reflection coefficient can be determined by more flexible ways using a suitable choice of possible measurements of reflectivity and polarization of the reflected beam. A schematic example is presented to illustrate the method.

PACS. 61.12.Ha Neutron reflectometry

1 Introduction

Cold and ultracold neutron specular reflection experiments are potentially powerful tools to probe the physics of many surfaces and interfacial microstructures of condensed matter [1–5]. In these experiments, the reflectivity profile $R(q)$ of a flat film sample, where $q = 2\pi \sin\theta/\lambda$, in terms of the neutron wavelength λ and the reflection angle θ, is measured to obtain information about the atomic or magnetic density profile of the sample along its depth.

However, the reconstruction of the surface profile has been hampered because of the so-called phase problem which has a long history in others fields such as optics and crystallography [6,7]. This problem refers to the fact that in reflection experiments only the square of the complex reflection coefficient, $R(q) = |r(q)|^2$, is measured and as any other scattering technique the phase of reflection is lost [8]. In the absence of the phase, generally least-squares methods are used to extract the scattering length density (SLD) depth profile [9,10] but in general more than one SLD may be found to correspond to the same reflectivity [11,12]. By using the phase and the reflectivity data, it is possible to solve the one-dimensional inverse scattering problem directly to obtain a unique SLD depth profile [13–15]. However, if the SLD profile is nowhere negative (i.e. supported potentials without bound states), Kramers-Kronig relations between the real and the imaginary parts of the reflection coefficient ensure that the inversion is unique and either the real or the imaginary part of $r(q)$ provides sufficient data [16].

Several methods for measuring the phase have been explored in neutron reflectometry [17–25]. Among these methods, however, the reference layer method first proposed in references [17,18] seems the most attractive because of its experimental application which was first achieved with good success by Majkrzak et al. [25], who also proposed and tested experimentally the related surrounding method [27,28].

The reference layer method based on using a magnetic reference layer for a polarized incident neutron beam and explicit polarization measurements instead of reflectivity, has been proposed by Leeb et al. and discussed in several works [29–31]. This method is of particular interest because it also works in the total reflection regime, and allows unique reconstruction of surface profiles of magnetic or absorptive nonmagnetic media. In this method, by using a magnetic reference layer mounted on top of the unknown layer, the polarization measurements rather than the reflectivity of the reflected beam are used to determine the phase of the reflection coefficient when the incident beam polarization is non-collinear to the magnetization

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of the reference layer (i.e. the polarization of the incident beam can be in any direction, but not parallel to the magnetization of the magnetic reference layer). However, the formalism of reference [29] is not applicable when the magnetic reference layer and the unknown layer are interchanged due to the fact that the wave function for scattering "from the left" by a sample on a substrate of finite thickness can be expressed in terms of corresponding "left" and "right" scattering functions for a bulk substrate [14]. In this case, they have shown that the reflection coefficient from the right of an absorptive unknown layer can be determined by using two sets of measurements with different layers [32].

In this paper we show that the transfer matrix method can be used to determine the complex reflection coefficient of an unknown sample mediated between the reference layer and the substrate by measuring the polarization of the reflected beam. Because of using the transfer matrix method, the method does not work in the total reflection regime. However, using the transfer matrix elements of the reference layer as known parameters, instead of the reflection and transmission coefficients of the entire sample without the unknown layer, is one of the advantages of the method. It is due to the fact that against the reflection and transmission coefficients, which depend strongly on the incident and transmitted media, the transfer matrix elements are independent of the surrounded media since in the transfer matrix method, the substrate and the media in front are included by the refractive index. This method for an incident beam fully polarized normal to the sample surface, has been investigated in references [33,34]. In these papers, we show that in all suitable ways for phase determination, measuring the polarization of the reflected beam parallel to the sample surface and normal to the magnetization of the reference layer is essential. However, in this paper we do not limit ourselves to a fully polarized incident beam and generalize the theory to a neutron polarization of arbitrary direction. It is shown that in this case some combination of the polarization of the incident and reflected beams should be used to determine the reflection coefficient. Also, apart from measurements of the final polarization orientation (i.e. only analyzing the results of the polarization measurements), we show that if provided with knowledge of the reflectivity of the reflected beam, a suitable choice of polarization and reflectivity measurements can be used to determine the phase. In this case, against the method of reference [29], in which the knowledge of the reflectivity must be considered after finding two possible solutions for reflection coefficient with final polarization orientation measurement, we show that measurement of two polarization components is sufficient.

The layout of the paper is as follows: In Section 2 we derive the basic relations between the reflectivity and the polarization of the reflected beam as functions of the transfer matrix elements for known and unknown layers and the refractive index of surrounding media. We show that three known parameters which depend on the polarization of the incident and reflected beam can be used to determine the complex reflection coefficient. In Section 3 we investigate the methods of phase determination and illustrate them with a computer simulation.

2 Determination of the polarization of the reflected beam as functions of transfer matrix elements

To derive the formalism of the method, we need the relations between the polarization of the reflected beam and the elements of the transfer matrix. We adopt the terminology that the incident and transmitting media are referred to as "fronting" and "backing" respectively, regardless of which mechanically supports the film, when the surrounding media is non vacuum fronting and backing, having constant SLD ρ_f and ρ_h, respectively. Thus, the complex reflection coefficient $r(q)$, can be written, with q suppressed, as

$$r(q) = \frac{\beta^{fh} - \alpha^{fh} - 2i\gamma^{fh}}{\alpha^{fh} + \beta^{fh} + 2}, \tag{1}$$

where "fh" as superscript indicates that the sample is surrounded by non vacuum fronting and backing and

$$\begin{aligned} \alpha^{fh} &= hf^{-1}A^2 + (fh)^{-1}C^2 \\ \beta^{fh} &= fhB^2 + fh^{-1}D^2 \\ \gamma^{fh} &= hAB + h^{-1}CD \end{aligned}, \tag{2}$$

where

$$n = (1 - 4\pi\rho_n/q^2)^{1/2}, \tag{3}$$

for n="f" and "h". The four real functions, $A(q), \ldots, D(q)$, uniquely determined by the scattering length density, ρ, of the film, are the elements of the 2×2 transfer matrix which carries the exact wave function and its first derivate across the film, from edge to back. Explicitly,

$$\begin{pmatrix} 1 \\ i \end{pmatrix} te^{iqL} = \begin{pmatrix} A(q) & B(q) \\ C(q) & D(q) \end{pmatrix} \begin{pmatrix} 1+r \\ i(1-r) \end{pmatrix} \tag{4}$$

where the column matrices contain the transmission and reflection coefficients, t and r, characterizing the wave function and its derivative in backing and fronting, respectively. L is the film thickness and q is the component of the incident wave vector normal to the sample surface. The directly measured reflection amplitude, $R(q)$, of the entire sample film and surrounding can be related to the three quantities in equation (2) in terms of the new quantity $\Sigma(q)$,

$$\Sigma(q) = 2\frac{1+R}{1-R} = \alpha^{fh} + \beta^{fh}. \tag{5}$$

For vacuum fronting or backing $n(q) = 1$, as appropriate. The critical q value, q_c, is defined by $q_c = Max(\rho_f, \rho_h)$, so that $f(q)$ and $h(q)$ are real valued for $q > q_c$, when ρ_f and ρ_h are real, corresponding to the absence of neutron absorption. The imaginary part of the scattering length density, which is negligible for neutrons, and for incoherent scattering, can generally be ignored for thin films, even when incoherent scattering such as with water are involved. Many methods use this advantage, like the reference layer method proposed by Majkrzak et al. [17,25,27]. It is assumed from here on that absorption in all film materials, as well as in the surrounding, is negligible. Thus, this method like the others which use this advantage, is not useful for some elements, such as Gd, Sm, B and Cd. An important consequence of this assumption is that the transfer matrix elements and the three quantities defined in equation (2) are real-valued at all q. We can see at once from equation (5) that at a given $q > q_c$, $R(q)$ contains less information than $r(q)$, an alternative perspective of the phase problem.

Now we consider that the composite film is separated into two distinct regions representing unknown and known parts. If the unknown sample is mounted on top of the known layer, the total transfer matrix can be expressed as a product of the corresponding transfer matrices

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} w & x \\ y & z \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{6}$$

where the matrix $(a, \ldots, d)$ describes the contribution from the unknown part of ρ and $(w, \ldots, z)$ gives the known part, i.e. the magnetic reference layer. Using equations (2) and (6), the three real quantities for composite films can be written as:

$$\begin{array}{l} \alpha = \alpha_k^{fh} a^2 + \beta_k^{fh} f^{-2} c^2 + 2\gamma_k^{fh} f^{-1} ac \\ \beta = \alpha_k^{fh} f^2 b^2 + \beta_k^{fh} d^2 + 2\gamma_k^{fh} f\, bd \\ \gamma = \alpha_k^{fh} hab + \beta_k^{fh} h^{-1} cd + \gamma_k^{fh} (ad + bc) \end{array}, \tag{7}$$

where "k" indicates the known portion of the composite film. Then, by using equation (5) we have

$$\Sigma(q) = \beta_k^{fh} \tilde{\alpha}_u^{ff} + \alpha_k^{fh} \tilde{\beta}_u^{ff} + 2\gamma_k^{fh} \tilde{\gamma}_u^{ff}, \tag{8}$$

where the subscript "u" refers to the unknown portion of the composite film, the tilde denotes a reversed film, that is, the interchange of the diagonal elements of the corresponding transfer matrix $a \leftrightarrow d$ [35], and "ff" refers to the same fronting and backing having constant SLD of ρ_f.

We consider a polarized incident beam and a magnetic field B within the magnetic reference layer which is directed in the z-direction as the direction of spin quantization (also, we assume the x-direction as the direction normal to the sample surface. Thus, z is perpendicular to the scattering vector and in the plane of the scattering and y is normal to the plane of scattering). Simply, the (x, y, z) coordinate system is just a standard Cartesian coordinate set. For a magnetic film, when the magnetization is in the plane of the film, three SLDs for a polarized incident beam can be obtained. For spin-up and spin-down incident neutrons, the SLD of the reference layer are $\rho = \rho_n \pm \rho_m$, respectively, where ρ_n is the nuclear scattering length density and ρ_m is the magnetic SLD of the reference layer. The third value, $\rho = \rho_n$, can be obtained from a demagnetized layer or with the magnetization perpendicular to the plane of the film. The magnetization of the magnetic layer will also generate magnetic induction outside the ferromagnetic film which we assume to be small enough not to affect the neutron beam.

As the SLD of the reference layer changes, α, β, and γ are different corresponding to the polarization of the incident beam. We consider $(w_\pm, \ldots, z_\pm)$ as the elements of the transfer matrix for the reference layer and $\alpha_{k\pm}^{fh}$, $\beta_{k\pm}^{fh}$ and $\gamma_{k\pm}^{fh}$ for the entire sample without unknown layer, where $\pm$ denotes up and down polarization of the incident beam (or plus and minus magnetization). Also we use $R_\pm$, $r_\pm$ and $\Sigma_\pm$ for the entire sample corresponding to plus and minus magnetization.

Now the polarization of the reflected beam, p_x, p_y, and p_z as functions of the elements of the transfer matrix of known and unknown layers is determined. We use the relation between the polarization of the reflected beam (p_x, p_y, and p_z), and the reflection coefficients, $r_\pm$, as follows

$$p_x + ip_y = \frac{2r_+^* r_- (p_x^0 + ip_y^0)}{R_+(1 + p_z^0) + R_-(1 - p_z^0)}, \tag{9}$$

$$p_z = \frac{R_+(1 + p_z^0) - R_-(1 - p_z^0)}{R_+(1 + p_z^0) + R_-(1 - p_z^0)}, \tag{10}$$

where p_x^0, p_y^0 and p_z^0 are the polarization of the incident beam.

The appearance of the product $r_+^* r_-$ in equation (9) arises from the interference between the two spin components of the neutron wave function and causes complicated formulae for p_x and p_y which are not useful in finding the unknown parameters by using the polarization of the reflected beam. However, instead of using p_x, p_y and p_z as known parameters to determine the unknown parameters, we suggest using the following relations, equations (11–13), which determine completely the unknown parameters. These relations can be obtained by using equations (1), (5), (8–10), after some straightforward (yet tedious) algebra.

$$\frac{p_x p_x^0 + p_y p_y^0}{p_{x^0}^2 + p_{y^0}^2} = 1 + 2\frac{\zeta_k - p_z^0(\Sigma_+ - \Sigma_-)}{\Sigma_+\Sigma_- + 2p_z^0(\Sigma_+ - \Sigma_-) - 4}, \tag{11}$$

$$\frac{p_x p_y^0 - p_y p_x^0}{p_{x^0}^2 + p_{y^0}^2} = \frac{2(c_{\beta\gamma}\tilde{\alpha}_u^{ff} + c_{\gamma\alpha}\tilde{\beta}_u^{ff} + c_{\beta\alpha}\tilde{\gamma}_u^{ff})}{\Sigma_+\Sigma_- + 2p_z^0(\Sigma_+ - \Sigma_-) - 4}, \tag{12}$$

$$p_z - p_z^0 = \frac{2(1 - p_{z^0}^2)(\Sigma_+ - \Sigma_-)}{\Sigma_+\Sigma_- + 2p_z^0(\Sigma_+ - \Sigma_-) - 4}, \tag{13}$$

where

$$\zeta_k = 2(1 + \gamma_{k+}^{fh}\gamma_{k-}^{fh}) - (\alpha_{k+}^{fh}\beta_{k-}^{fh} + \beta_{k+}^{fh}\alpha_{k-}^{fh}), \tag{14}$$

and

$$c_{ij} = i_{k+}^{fh} j_{k-}^{fh} - j_{k+}^{fh} i_{k-}^{fh}, \tag{15}$$

for "i" and "j"= α, β, and γ.

It is obvious that ζ and c_{ij} are known parameters since they are independent of the unknown layer. Using equations (11–13), one can find that aside the dominator, the

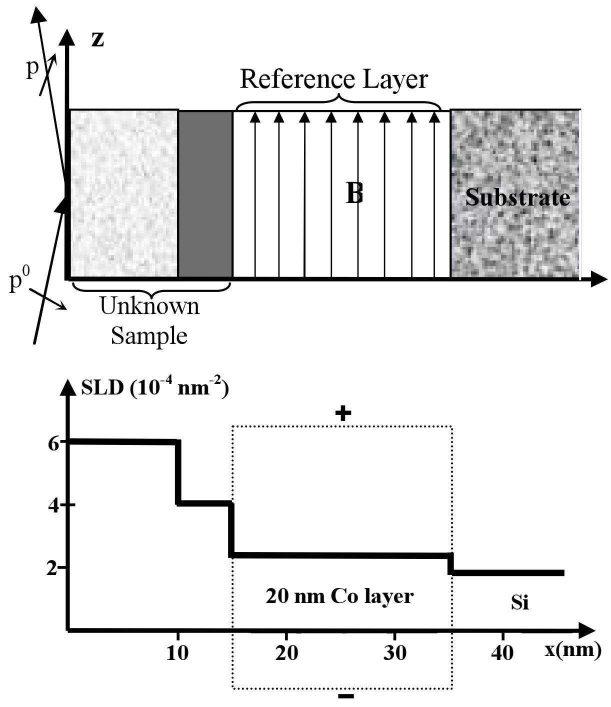

Fig. 1. Experimental arrangement to test the method of complex reflection coefficient determination. Top: Arrangement of the layers. Bottom: the SLD depth profile of the layers. The dotted lines represent the effective SLD's experienced by neutron beams polarized parallel or antiparallel to the magnetic field.

difference between the components of the polarization of the reflected and incident beam in x, y and z directions, dependence to the unknown parameters by linear combinations.

3 Phase determination

Equations (11–13) are the basic formulae for our method of determining the phase. These formulae enable us to determine the unknown parameters (i.e. the parameters characterized by subscript "u") by more flexible methods. These methods are illustrated by a computer simulation. In this simulation, we consider an arrangement containing a 20 nm thick magnetized Co film as the reference layer, and a bilayer sample having constant SLD values of 6×10^{-4} nm^{-2} and 4×10^{-4} nm^{-2} with 10 and 5 nm thickness, respectively. The effective SLD's experienced by neutron beams polarized parallel or antiparallel to the magnetic field in the Co layer are 6.44×10^{-4} nm^{-2} and -1.98×10^{-4} nm^{-2}, respectively. We assume a Si wafer as the substrate and the incident medium is assumed to be vaccum. The arrangement is similar to that studied by Leeb et. al [29], except that we have interchanged the position of the sample and the reference layer.

Now, we investigate equations (11–13) depending on the polarization of the incident beam.

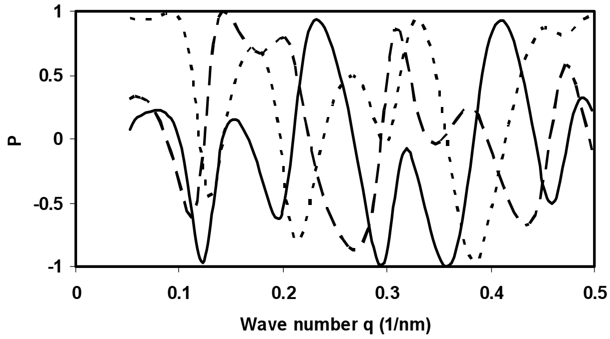

Fig. 2. Simulated polarization data of the reflected beam for the arrangement of Figure 1, for q greater than q_c. The incident beam is assumed to be polarized as $p_x^0 = 0.6$, $p_y^0 = 0.8$, and $p_z^0 = 0.0$. The polarization components: p_x (dotted), p_y (dashed) and p_z (solid).

3.1 Incident beam with specific polarization

Consider that we measure the polarization of the reflected beam for the case that the incident beam is polarized out of the magnetization of the reference layer. The dependence on unknown parameters in equations (11) and (13), is encoded in the parameters Σ_+ and Σ_-. This dependence lets us determine Σ_+ and Σ_- by using the polarization of the incident and reflected beams, as follows

$$\Sigma_{\pm}^2 \mp \frac{\zeta_k}{\zeta_p}\Sigma_{\pm} - \left(4 + 2\frac{\zeta_k(1 - p_z p_z^0)}{\zeta_p(p_z - p_z^0)}\right) = 0, \qquad (16)$$

where

$$\zeta_p = p_z^0 + \frac{1 - p_{z^0}^2}{p_z - p_z^0}\left(\frac{p_x p_x^0 + p_y p_y^0}{p_{x^0}^2 + p_{y^0}^2} - 1\right). \qquad (17)$$

ζ_p is an experimentally obtainable quantity since it depends only on the polarization of the incident and reflected beams. As equation (16) has two solutions, the physical solution can be selected by requiring that $\Sigma_\pm$ must satisfy $\Sigma_\pm \geq 2$, corresponding to $R_\pm \leq 1$. By knowing Σ_+ and Σ_-, we have two linear equations for unknown parameters, equation (8), and a third equation can be found by using equation (12). Thus the unknown parameters can be determined as follows:

$$\begin{pmatrix} \tilde{\alpha}_u^{ff} \\ \tilde{\beta}_u^{ff} \\ \tilde{\gamma}_u^{ff} \end{pmatrix} = \begin{pmatrix} \beta_{k+}^{fh} & \alpha_{k+}^{fh} & 2\gamma_{k+}^{fh} \\ \beta_{k-}^{fh} & \alpha_{k-}^{fh} & 2\gamma_{k-}^{fh} \\ c_{\gamma\beta} & c_{\alpha\gamma} & c_{\alpha\beta} \end{pmatrix}^{-1} \begin{pmatrix} \Sigma_+ \\ \Sigma_- \\ \frac{\zeta_k(p_x p_y^0 - p_y p_x^0)(1 - p_{z^0}^2)}{\zeta_p(p_z - p_z^0)(p_{x^0}^2 + p_{y^0}^2)} \end{pmatrix}. \qquad (18)$$

To simulate equations (16) and (18), we assume $p_x^0 = 0.8$, $p_y^0 = 0.6$, and $p_z^0 = 0$ for the polarization of the incident beam. The polarization of the reflected beam in this case, for q greater than q_c, is shown in Figure 2. By using the data of Figure 2, two possible solutions for R_+ and R_-, according to two solutions of equation (16) for $\Sigma_\pm$ of the arrangement of Figure 1, can be obtained which are shown in Figure 3.

It is obvious that only one of the solutions satisfies the physical condition, $R_\pm \leq 1$. Using these two physical

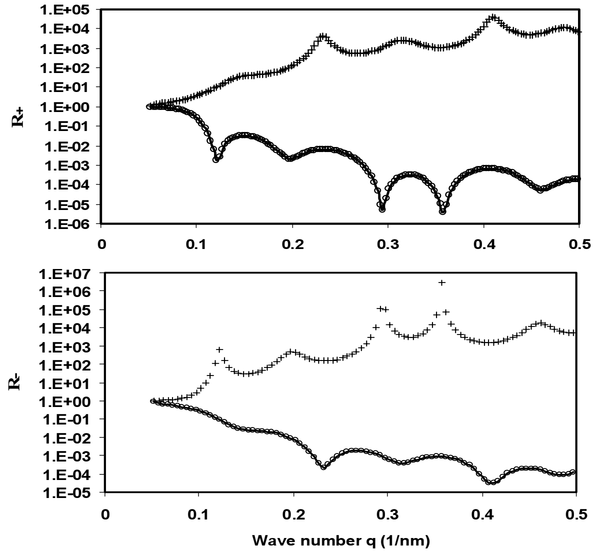

Fig. 3. Two solutions (circles and pluses) of R_- and R_+, corresponding to two solutions for $\Sigma_\pm$ recovered from p_x and p_y, by using equation (16) for q greater than q_c. Solid lines: R_- and R_+ computed directly from equation (5).

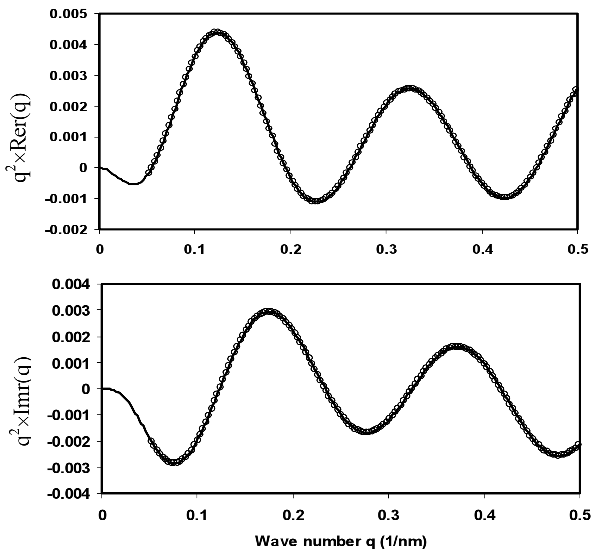

Fig. 4. $q^2 \times \mathrm{Re}r(q)$ and $q^2 \times \mathrm{Im}r(q)$ for the mirror image of the unknown sample of Figure 1. Solid line: computed directly from equation (1). Circles: Recovered by using two physical reflectivities in Figure 3, p_y in Figure 2 and equation (18) for q greater than q_c .

solutions in equations (18) and (19), the reflection coefficient for the reversed unknown sample $\tilde{r}(q)$ (the incident medium is vacuum) can be determined as shown in Figure 4.

Use the fact that $\Sigma_\pm \geq 2$, for solving the problem of selecting a physical solution between the two solutions of equation (16), seems reasonable since for q values above q_c only one root satisfies the condition $\Sigma_\pm \geq 2$, as shown in Figure 3. However, this is seen for many numerical simulations and there is no general proof for this [30].

To avoid this problem, we suggest using a combination of the polarization and reflectivity measurements on the reflected beam. Since we want to measure the reflectivity, we have to change the polarization of the incident beam and consider an incident beam polarized parallel or antiparallel to the direction of magnetic field.

3.2 Incident beams with two different polarizations

To avoid having two solutions or a complex solution of equation (16), we suggest using two incident beams, one being polarized out of the magnetization direction of the reference layer and the other parallel or antiparallel to it. Application of the reflectivity to solve the problem of selection of the physical solution has been proposed by Leeb et al. [30] too, however, in that case it is necessary to find two solutions and to use the reflectivity as additional information. In our method, we show that by knowing the reflectivity, the final polarization orientation measurement is not necessary.

Assume we measure either R_+ or R_-, when the incident beam is polarized parallel or antiparallel to the magnetic filed, respectively. Equations (11) and (13) show that the other one can be deduced by measuring two of the three parameters of the polarization; p_x, p_y, and p_z, when the incident beam is polarized non-collinear to the direction of magnetic field. Thus, we have six possible ways to determine the data of (Σ_+, Σ_-, p_y) to use in equations (18) and (19) in order to find the unknown parameters.

In the case that we do not measure p_y directly (that means p_x, p_z and either R_+ or R_- are measured), it can be determined by using equation (11). However, for an incident beam non-polarized in the y direction, $p_y^0 = 0$, this is impossible since p_y disappears from the left side of equation (11). Thus for an incident beam non-polarized in the y or x direction, the six possible methods reduce to four ways. For these cases, equation (12) shows that measuring p_x (p_y) for an incident beam which is fully polarized in the $y(x)$ direction is necessary. Nevertheless, using an incident beam fully polarized in the x or y direction, equations (11–13) and (17) are simpler. As an example, consider that the incident beam is fully polarized in the $+y$ direction (i.e. $p_x^0 = 0$, $p_y^0 = 1$, and $p_z^0 = 0$). Thus, equations (11–13) and (17) reduce to

$$p_x = \frac{2(c_{\gamma\beta}\tilde{\alpha}_u^{ff} + c_{\alpha\gamma}\tilde{\beta}_u^{ff} + c_{\alpha\beta}\tilde{\gamma}_u^{ff})}{\Sigma_+\Sigma_- - 4}, \tag{19}$$

$$p_y = 1 + \frac{2\zeta_k}{\Sigma_+\Sigma_- - 4}, \tag{20}$$

$$p_z = \frac{2(\Sigma_+ - \Sigma_-)}{\Sigma_+\Sigma_- - 4}, \tag{21}$$

$$\zeta_p = (p_y - 1)/p_z. \tag{22}$$

Equation (20) shows that measuring p_x is necessary in this case. To illustrate the case, we consider the situation that (R_+, p_x, and p_z) are measured. By using the data of R_+, in Figure 3, and p_z, in Figure 2, R_- can be determined very simply by using equation (22), as shown in Figure 5,

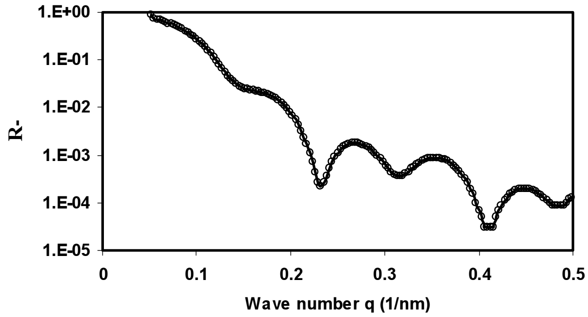

Fig. 5. The data for R_- recovered using R_+ and p_z for the arrangement shown in Figure 1. Solid line: Σ_- computed directly using equations (1) and (5).

in which the recovered data is compared to Σ_- computed directly by using equations (5) and (1). The stability of the phase reconstruction by this method, in the presence of experimental uncertainties and the surface roughness, has been investigated in reference [34].

3.3 Incident beams with three different polarizations

As mentioned before, by knowing Σ_+, Σ_- and measuring either p_x or p_y, three linear equations can be obtained for three unknown parameters. We showed in the two previous subsections how Σ_+ and Σ_- can be determined by different flexible ways. However, it is obvious that these two parameters can be measured directly. Thus if we use three incident beams polarized parallel, antiparallel and non-collinear to the magnetic field and measure Σ_+, Σ_- and either p_x or p_y, respectively, we can determine the unknown parameters.

Once three parameters $\tilde{\alpha}_u^{ff}$, $\tilde{\beta}_u^{ff}$ and $\tilde{\gamma}_u^{ff}$ are determined, the complex reflection coefficient of the mirror-reversed unknown film surrounded on both sides by a uniform medium of SLD ρ_f is determined. The reflection coefficient below the critical q_c, for total external reflection can be determined by considering the fact that $\text{Re}r(q) \to -1$ and $\text{Im}r(q) \to 0$, as $q \to 0$. Since the reflection coefficient is known in amplitude and phase, the transformation $r(q) \to \rho$ can be performed in a straightforward way, with the help of the Gel'fand-levitan integral equation. This SLD profile is equivalent to a reversed free film SLD profile, $\tilde{\rho}_{equiv}(z)$, defined by

$$\tilde{\rho}_{equiv}(z) = \rho(z) - \rho_f, \tag{23}$$

which behaves as if it is against a backing having relative index of refraction $h(q)/f(q)$. So by knowing the SLD of a mirror reversed free unknown film, the SLD of the free unknown film can be extracted taking $\tilde{\rho}_{equiv}(z) \equiv \rho(L-x)$, where L is the width of the unknown film. Our example, Figure 6, shows that the reconstructed SLD depth profile using the data of Figure 4 (The data below q_c has been determined by considering $r(q) \to 1$). As is seen, the reconstructed SLD is exactly the SLD of the mirror image of the unknown layer in Figure 1. This is due to the fact that in our example the incident beam is assumed to be in a vaccum.

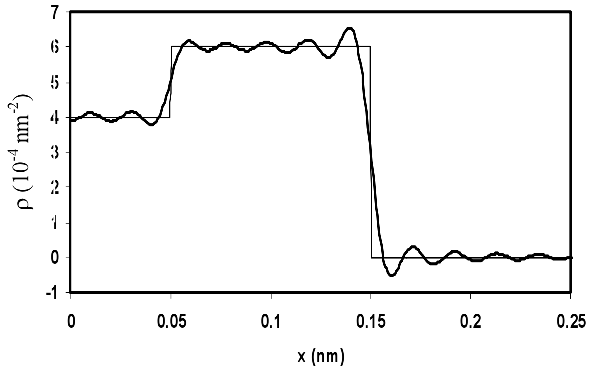

Fig. 6. The reconstructed SLD of the unknown sample in Figure 1, obtained by inversion of the extracted values of the reflection coefficient in the momentum range $0 \le q \le 1.5\ \text{nm}^{-1}$. The original profile is shown by thin solid lines.

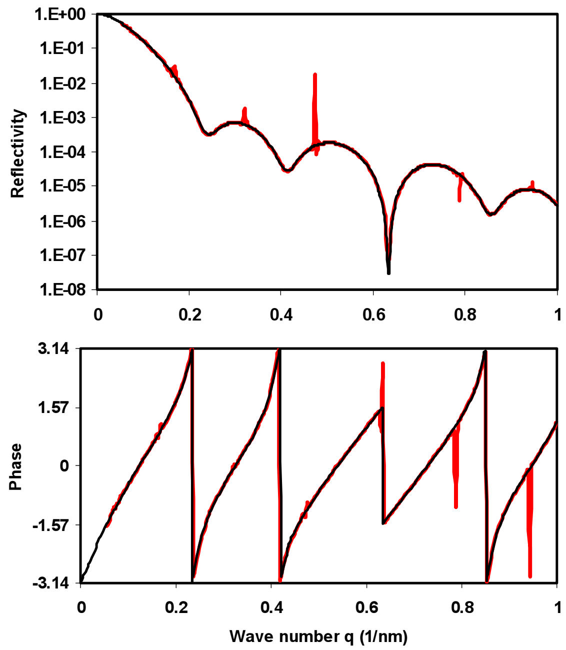

Fig. 7. Effect of measurement errors on the extraction of the reflectivity and the phase of the reflection coefficient of an unknown sample for the arrangement shown in Figure 1. The simulation includes 2% and 1% statistical errors in the input data of the polarization of the reflected and incident beams, respectively.

4 Stability of the method

So far we have used exact data, and therefore the recovered data must be perfect, as Figure 4 shows. To test the resolution of the method in the presence of experimental uncertainties, we consider an error of 2% and 1% statistical errors in the accuracy of measuring the polarization of the reflected and incident beams, respectively (1% error refers to the measured polarization direction being accurate to ~3 degrees). By using this statistical ensemble of data as input, we reconstruct the amplitude and the phase of the reflection coefficient as displayed in Figure 7, where the exact complex reflection coefficient is shown as well.

This figure shows that the results are in good agreement with the exact values, and the method is tolerant against such errors.

5 Conclusion

We have presented a method to determine the complex reflection coefficient in neutron specular reflectometry. It exploits the interference of the spin components of a polarized neutron beam in the presence of a magnetic reference layer mediated between substrate and sample. The method is based on the transfer matrix formalism and requires polarization analysis of the reflected beam. However, in addition to final polarization orientation measurement, it is shown that a suitable choice of polarization and reflectivity measurements can also be used to determine the reflection coefficient. The method is supplemented with a specific example. Finally, it has been shown that the method is stable against possible experimental uncertainties

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