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Superpolarizing neutron coatings: Theory and first experiments

N.K. Pleshanov *

Petersburg Nuclear Physics Institute, 188300 Gatchina, St. Petersburg, Russia

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A B S T R A C T

A new method for improving polarizing neutron coatings is theoretically substantiated and experimentally verified. It is based on the use of layers with a negative potential of definite thickness to suppress reflection of neutrons with the undesired spin from the potential barriers formed by structural imperfections. Estimations showed that Ti, Co or Ti/Co interlayers at the interfaces and a protective Ti/TiO_2 surface bilayer may increase the flipping ratio for reflection from polarizing neutron coatings by orders of magnitude. It opens the possibility to build polarizers and analyzers of new generation. *Superpolarizing* coatings not only will improve the performance and thus widen the range of applications of the polarizing devices, but also may be the basis for designing novel neutron instrumentation. Even ultra-cold neutron beams can be efficiently polarized and analyzed with new polarizing neutron optics. A method for precise measurements of NSF and SF reflectivities of the spin-down neutrons for polarizing coatings with the flipping ratios up to 10^3–10^4 is suggested (method of two samples).

1. Introduction

Polarized neutrons are known to be a unique probe allowing important physical information to be obtained, inaccessible by other experimental techniques. This information had a great impact in many fields of science and technology. An increase in the polarizing efficiency of neutron polarizers and analyzers means more direct, detailed and reliable information in experiments with polarized neutrons. Quite often, to achieve a reasonable resolution, polarized neutron beams with relatively small divergence are required and the polarization of scattered neutrons is analyzed with numerous channels of small angular aperture. Then neutron optical polarizers [1,2] may turn out to be more efficient than ^{3}He spin filters [3,4] and their development remains an important task.

To increase the angular acceptance and the transmittance of the neutron optical polarizers, supermirror coatings [5] are used. Thicknesses of layers in a supermirror are gradually changed to reflect neutrons at glancing angles up to an angle, in m times exceeding the total reflection edge of Ni, one of the best neutron reflectors. Polarizing supermirrors are built by alternating magnetic and non-magnetic layers with a low neutron optical contrast for one of the spin components. The substrate is coated with an absorbing antireflective underlayer [6] (we do not consider transmission polarizers without underlayers; their polarizing efficiency cannot be noticeably improved by the methods suggested in the present paper). The composition and the thickness of the underlayer can be designed to minimize reflection to any reasonable level [7]. By using efficient underlayers and matching the potentials of non-magnetic and magnetic layers, the spectral reflectivities for neutrons with the spin opposite to the magnetization of the magnetic layers (spin-down neutrons) are reduced to a level about 1%, e.g., for CoFe(V)/TiZr [2] and CoFeV/TiN [8] supermirrors.

Among the remaining factors that enhance reflection of the spin-down neutrons are structural imperfections, including an oxide layer on the supermirror surface [9] and “magnetically dead” regions [10,11] in magnetic layers near interfaces, that give rise to appearance of the potential barriers for neutrons with the undesired spin. The origin of the “magnetically dead” regions with a zero mean magnetization is a roughness-induced spin-orientational disorder. A sequence of the demagnetized interfacial regions forms numerous potential barriers, which reflect the spin-down neutrons and worsen the polarizing efficiency of the supermirrors.

Thus, in Ref. [12] a satisfactory and consistent fitting of both spin-up and spin-down neutron reflectivities of a polarizing CoFe/TiZr supermirror was obtained with a model, taking account of the roughness and the law of its growth from interface to interface, a difference in structural and magnetic roughness, the presence of demagnetized interfacial regions and the surface oxide layer. Particularly, it was shown that the difference in magnetic and structural roughness noticeably enhances the spin-down neutron reflection from the sequence of the barriers. The

* Corresponding author. Tel.: +7 81371 46973; fax: +7 81371 39053.
E-mail address: pnk@pnpi.spb.ru

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model developed in Ref. [12] will be used to substantiate the suggested methods for improving the polarizing efficiency of neutron coatings.

The neutron reflectivity is a function of the wave vector transfer

$$q=\frac{4\pi\sin\theta}{\lambda}=\frac{\sqrt{8mE_0}\sin\theta}{\hbar}=\frac{\sqrt{8mE}}{\hbar}, \quad (1)$$

where m, λ and E_0 are the neutron mass, wavelength and energy, respectively, E is a fraction of the kinetic energy corresponding to the neutron velocity component normal to the surface and θ is the glancing angle. The particles with extremely small energies $E \ll V_b$ are known to be totally reflected from an isolated square potential barrier with a thickness b and a potential $V_b>0$. A detailed analysis [13] (its synopsis is represented in Appendix A) showed that reflection from a barrier or even many barriers can be efficiently suppressed by antireflective layers with a negative potential and of definite thickness. When the barrier is sufficiently thin ($bq_b<1$, $q_b=\sqrt{8mV_b}/\hbar$ is the critical wave vector transfer), a neighboring square potential well with a potential $V_a<0$ and a definite thickness a_0 may reduce reflection of such particles by orders of magnitude. Calculations showed that suppressing neutron reflection at extremely small wave vector transfers by means of such antireflective (antibarrier) layers, one obtains sufficiently low reflection in the entire range of q. Surrounding the barrier with two wells with a definite thickness, one can totally suppress reflection of the particles with energies $E \ll V_b$ from the barrier. The same is proven for multilayers built from such bilayers and trilayers. It holds true even when these bilayers and trilayers are separated by layers with a zero potential and arbitrary thicknesses.

Absorption, thickness errors and roughness impose restrictions on the efficiency of the antireflective layers. However, these restrictions are sufficiently mild [13]. Particularly, absorption increases the reflectivity only at $q<q''=\sqrt{8mV''}/\hbar$, where V''=max(|Im(V_a)|, |Im(V_b)|), i.e. at wave vector transfers by about 2 orders of magnitude lower than q_b. The effect of a thickness error Δa_0 is noticeable only at $q<1a(\Delta a_0/a_0)$, where $|q_a|=\sqrt{8m|V_a|}/\hbar$, i.e. also at very small wave vector transfers. The effect of roughness is even less significant, especially when we can correct the optimum thickness of the antireflective layer for roughness (Appendix A).

In Sections 2 and 3 the simulations, made with the numerical matrix method (e.g., see [14]), demonstrate the possibilities of the antireflective layers on the basis of Ti to suppress reflection of neutrons with the undesired spin from the surface oxide layer (Section 2) and demagnetized interfacial regions (Section 3) in polarizing neutron coatings. Layer thickness sequences of all supermirrors were generated by the real-structure algorithm [15]. We assume that the magnetization of each magnetic layer is parallel to the applied field. A high antireflective efficiency of Ti interlayers in polarizing supermirrors is confirmed by the experimental data (Section 4). The results are discussed in Section 5.

2. Suppression of reflection from the oxide layer

The interaction potentials of a ferromagnetic layer for neutrons in the states with the spin projection up (+), i.e. parallel to, and down (−), i.e. opposite to, the layer induction are $V_\pm=V_n\pm V_m$, where V_n and V_m are the nuclear and magnetic potentials. To minimize reflection of the spin-down neutrons, the composition of the ferromagnetic layer is such that the potential V_- is close to 0. However, a non-magnetic surface oxide layer forms in air and presents a barrier enhancing reflection of neutrons with the

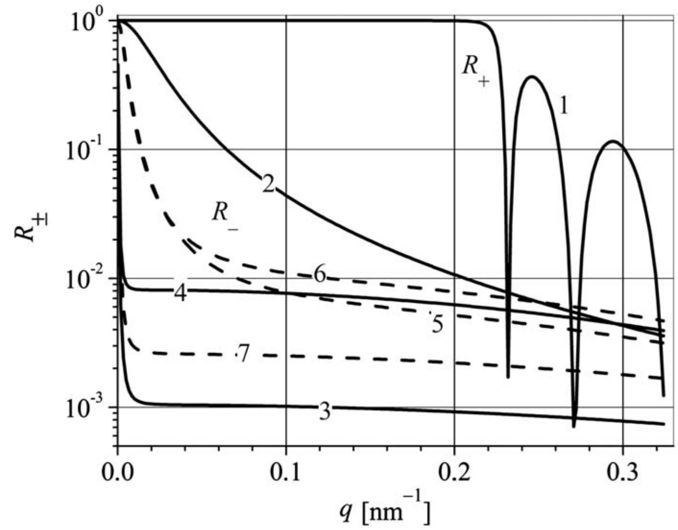

Fig. 1. The neutron reflectivities calculated as functions of the wave vector transfer q. Curve 1 (2) is R_+ (R_-) for a CoFe layer of thickness 75 nm and potential V_+=244 neV (V_-=0) and the surface oxide layer 3.5 nm thick. Curves 3–7 are the reflectivities R_- for the bilayers: (3) Ti(4.16 nm)/TiO_2(3 nm); (4) Ti(6.66 nm)/TiO_2(5 nm); (5) Ti(7.8 nm)/TiO_2(4 nm); (6) Ti(6.09 nm)/TiO_2(6 nm) and (7) Ti(5.4 nm)/Ag(3 nm).

undesired spin component. For example, according to neutron and X-ray reflectometry data, the thickness of the oxide layer on the surface of $Co_{68}Fe_{30}V_2$ [9] and $Co_{70}Fe_{30}$ [12] layers is 3.5 nm. Curve 1 in Fig. 1 is the spin-up neutron reflectivity R_+ calculated for a $Co_{70}Fe_{30}$ layer of thickness 75 nm. Curve 2 is the spin-down neutron reflectivity R_- for a single barrier (oxide layer) of thickness b=3.5 nm and height V_b=126 neV [12]. Bearing in mind that the underlayer can be designed to minimize its reflectivity to any reasonable level [7], the underlayer and the substrate were substituted by a half-space with a zero potential (to avoid their contribution into reflection). It will enable us to analyze the effect of other factors on the reflectivity R_-.

The barrier with b=3.5 nm and V_b=126 neV is sufficiently thin ($bq_b\cong 0.55$) and an adjacent layer with a negative potential (antireflective layer) can efficiently suppress neutron reflection from the barrier. Among a few elements with a negative neutron coherent scattering length, titanium (V_a=−49 neV) seems to be the most suitable. However, a layer of oxide, mostly routile TiO_2, which is formed on Ti film surface, also presents a barrier of height V_b=68 neV (its thickness b was found [16] to be less than 3 nm for a 100-nm Ti film). It is evident that the Ti layer deposited on the ferromagnetic film should be sufficiently thick to avoid its complete oxidation. For a deposited Ti layer of thickness

$$d=a_0+b/\varepsilon_{Ti} \quad (2)$$

where b is the thickness of the oxidized part of Ti and ε_{Ti}=1.76 [17] is the volume expansion coefficient for oxidation of Ti, the thickness a of the unoxidized part will be equal to a_0 given by Eq. (A.1), i.e. to the thickness optimal for suppression of reflection from the barrier formed by the TiO_2 layer. Note that the ferromagnetic film is now protected from oxidation by the Ti/TiO_2 bilayer.

Curve 3 is the neutron reflectivity for the Ti/TiO_2 bilayer with $a=a_0\cong 4.16$ nm and b=3 nm ($bq_b\cong 0.34$). It confirms the efficiency of the method. A sharp increase in the reflectivity at $q<0.02$ nm^{-1} is a ‘metallic’ reflection from an absorbing layer (as discussed in Introduction). The oxidation of very thin Ti layers and the stability of the oxide layers are still to be studied. Note that the reflectivity remains low (curve 4) even on the assumption that