Pis'ma v ZhETF, vol.63, iss.12, pp.900 - 905

OFF-SPECULAT NEUTRON REFLECTION FROM MAGNETIC MEDIA WITH NONDIAGONAL REFLECTIVITY MATRICES

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Submitted 6 May 1996

The reflection of neutrons from magnetic substances is described using the reflection matrix with nondiagonal, in general, matrix elements which determine neutron spin reverse. In external field the spin reverse is accompanied by changes of the neutron kinetic energy and, as results, the reflection angle. The experiment to observe this new effect is described and its results are reported.

PACS: 61.12.-q; 75.70.-i; 78.66.-w

Introduction. Since the time of the first works by Hughes and Burgy [1], specular reflection has been used to polarize neutrons. With polarized neutrons one can investigate, for instance, magnetization profiles of films and multilayered systems [2]. In general the reflection of neutron from magnetic mirror is characterized by the reflection matrix [3]:

$$\hat{R} = \begin{pmatrix} R_{++} & R_{+-} \\ R_{-+} & R_{--} \end{pmatrix}$$

with nonzero elements R_{+-} and R_{-+}. To measure all matrix elements in $\hat{R}$ is the main goal of polarized neutron reflectometry [4].

In the next section, the angular characteristics of reflection with spin-flip in external fields are considered. In the third section, the matrix elements of $\hat{R}$ and the intensities of constituent beams for the case of reflection from a magnetic mirror with magnetization noncollinear to the external field are calculated. In the fourth section, the experiment to observe off-specular reflection is described.

Angular splitting of the reflected beam. The reflection of neutrons from an interface in an external magnetic field can be off-specular (though coherent) if it is accompanied by spin flipping [5]. In general, the incident beam after reflection undergoes triple splitting, as shown in fig. 1. It contains the middle part which is specular and two side lobes which are off-specular and perfectly polarized. The intensity of the side lobes are determined by the matrix elements R_{+-} and R_{-+} of the matrix $\hat{R}$ and by the incident beam polarization. If the incident beam is perfectly polarized, one of the side lobes vanishes. If the incident beam is nonpolarized, two side beams in weak external fields have almost equal intensities. The splitting of the beam takes place because of spin flipping, energy conservation and the conservation of components of neutron momentum parallel to the interface.

Let us denote $\mathbf{k} = (\mathbf{k}_{\parallel}, k_{\perp})$ the wave vector of the incident neutron with $k_{\perp}$ and $\mathbf{k}_{\parallel}$ being its normal and parallel to surface components. In the external field

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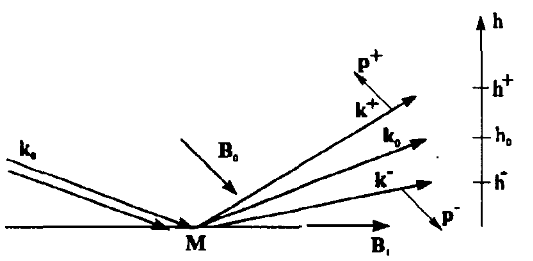


Fig.1. Following the reflection from a magnetized mirror with the magnetization **M** noncollinear to the external magnetic field B_0 the nonpolarized incident neutron beam with a wave vector k_0 splits into three beams. Two off-specular beams with the wave vectors k^+ and k^- are ideally polarized. The splitting of the beam gives the distribution over height h of the reflected neutrons and it can be measured by a moving or a position sensitive detector

B the neutron has the potential energy $-\sigma B$, where B is measured in $\hbar^2/2m\mu$ (m, μ are the neutron mass and magnetic moment, respectively) and σ are the Pauli matrices. On spin reverse the potential energy changes in magnitude by $\pm 2B$. Because of energy conservation it changes the kinetic energy: $k^2 \to k^2 \pm 2B$. In the reflection from an interface the components $\mathbf{k}_{\|}$ are also conserved. Thus the change of the kinetic energy means a change in the normal component $k_\perp$: $k_\perp \to k_\perp^\pm = \sqrt{k_\perp^2 \pm 2B}$, and as a result to change in the reflection angle. It is not difficult to calculate the angular deviation of shifted beams. For a small grazing angle $\phi_0 = 10^{-2} \div 10^{-3}$ rad we have

$$\frac{\Delta\phi^\pm}{\phi_0} = \frac{\Delta k_\perp^\pm}{k_\perp} = \sqrt{1 \pm 2B/k_\perp^2} - 1 = \sqrt{1 \pm 1.47 \cdot 10^{-10} B\lambda^2/\phi_0^2} - 1.$$

Here the neutron wave length λ is measured in Ängstroms, B in Gauss, and ϕ_0 — in radians. The dependence of the relative splitting $\Delta\phi^\pm/\phi_0$ on λ and B is shown in fig. 2. If the external field is sufficiently large, spin reverse is forbidden for $\Delta\phi < 0$.

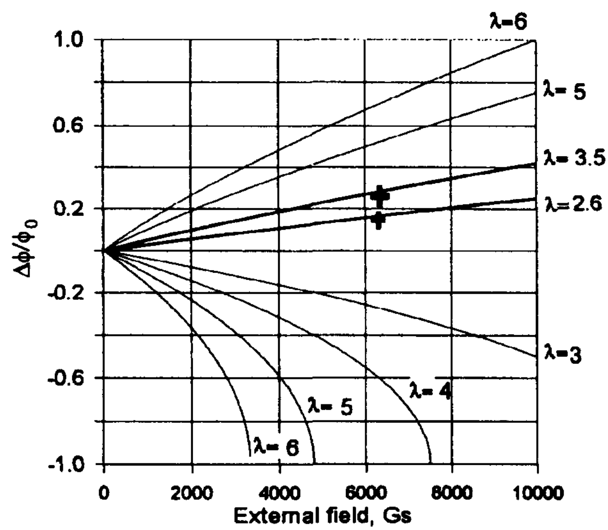


Fig.2. The relative angular splitting of spin reversed beams in dependence on λ (in Ängstroms) and the external magnetic field for $\phi_0 = 4.2$ mrd. The crosses are the experimental points (see sec. 4)

Matrix $\hat{R}$. Let us find the solution of the Schrödinger equation in the presence of the external magnetic field $\mathbf{B}_0$ and a magnetized reflecting mirror:

$$(\Delta - u\theta(z > 0) + \sigma\mathbf{B}(z) + k^2)\psi = 0, \tag{1}$$

where u is an optical potential of the mirror, which is supposed to fill the half space $z > 0$, θ is the step function equal to unity when the inequality in its argument is satisfied and to zero in the opposite case,

$$\mathbf{B}(z) = \mathbf{B}_0\theta(z < 0) + \mathbf{B}_1\theta(z > 0),$$

and $\mathbf{B}_1$ is the magnetic induction of the mirror. We consider the particular case when $\mathbf{B}_0 \not\parallel \mathbf{B}_1$. The solution is $\psi(\mathbf{r}) = \exp(i\mathbf{k}_{\parallel}\mathbf{r}_{\parallel})\xi(z)$, where

$$\begin{aligned} \xi(z) &= \theta(z < 0)[\exp(i\hat{k}_{\perp}^{+}z)\xi_0 + \exp(-i\hat{k}_{\perp}^{+}z)\hat{R}\xi_0] + \\ &+ \theta(z > 0)\exp(i\hat{k}_{\perp}'^{+}z)\hat{T}\xi_0, \end{aligned} \tag{2}$$

$\hat{R}$, $\hat{T}$ are the reflection and transmission matrices, $\hat{k}_{\perp}^{\pm} = \sqrt{k_{\perp}^2 \pm \sigma\mathbf{B}}$, $\hat{k}_{\perp}'^{\pm} = \sqrt{k_{\perp}^2 - u \pm \sigma\mathbf{B}}$ and ξ is the spinor state of the incident particle. For simplicity in the following, we shall omit the subscript $\perp$.

Matching of the wave function at the interface $z = 0$ for arbitrary ξ_0 gives two equations for $\hat{R}$ and $\hat{T}$:

$$\hat{I} + \hat{R} = \hat{T}, \qquad \hat{k}^{+}(\hat{I} - \hat{R}) = \hat{k}'^{+}.$$

The solution of these equations can be represented as follows:

$$\hat{R} = (\hat{k}^{+} + \hat{k}'^{+})^{-1}(\hat{k}^{+} - \hat{k}'^{+}), \quad \hat{T} = (\hat{k}^{+} + \hat{k}'^{+})^{-1}2\hat{k}^{+}.$$

Here we shall consider in details only the matrix $\hat{R}$.

It is possible to get rid of the matrices σ in the denominator by representing $\hat{R}$ in the form

$$\hat{R} = (\hat{k}^{-} + \hat{k}'^{-})(\hat{k}^{+} - \hat{k}'^{+})/N \equiv \hat{A}/N, \tag{3}$$

where N is the number, and it is useful to calculate it as a matrix element:

$$N = < +|k^{+}k^{-} + \hat{k}'^{+}\hat{k}'^{-} + \hat{k}'^{-}k^{+} + k^{-}\hat{k}'^{+}|+ >,$$

where $|\pm>$ represent the eigen states of the matrix $\sigma\mathbf{B}_0$:

$$f\sigma\mathbf{B}_0|\pm> = \pm B_0|\pm> .$$

Evaluation gives

$$N = (k^{+} + k'^{+})(k^{-} + k'^{-}) - (k'^{-} - k'^{+})(k^{+} - k^{-})\sin^2(\chi/2) \tag{4}$$

where $k^{\pm} = \sqrt{k^2 \pm B_0}$ and $k'^{\pm} = \sqrt{k^2 - u \pm B_1}$ are the c-numbers now, and χ is the angle between the vectors $\mathbf{B}_0$ and $\mathbf{B}_1$.

The numerator of (2) can be reduced to the form:

$$\begin{aligned} \hat{A} &= k^{-}k^{+} - k'^{-}k'^{+} + \hat{k}^{-}\hat{k}'^{+} - \hat{k}'^{-}\hat{k}^{+} = \\ &= k^{+}k^{-} - k'^{+}k'^{-} + (1/2)(k'^{-} + k'^{+})(\hat{k}^{+} - \hat{k}^{-}) - \\ &- (1/2)(k'^{+} - k'^{-})(\hat{k}^{-}\sigma\mathbf{b}_1 + \sigma\mathbf{b}_1\hat{k}^{+}), \end{aligned}$$

where the first two terms do not contain the σ matrices at all, and $\mathbf{b}_1$ is the unit vector in the direction of $\mathbf{B}_1$.

Now we can calculate the matrix elements of $\hat{A}$:

$$\begin{aligned} <\pm|\hat{A}|\pm> &= (k^- \pm k'^-)(k^+ \mp k'^+) \pm \\ &\pm\ (k'^+ - k'^-)(k^+ + k^-)\sin^2(\chi/2), \\ <\mp|\hat{A}|\pm> &= -(k'^+ - k'^-)k^{\pm}\sin\chi, \end{aligned}$$

In the case of $\chi = 0$ (and the similarly for $\chi = \pi$) the matrix $\hat{R}$ becomes diagonal with the elements $R_+ = (k^+ - k'^+)/(k^+ + k'^+)$, $R_- = (k^- - k'^-)/(k^- + k'^-)$.

For the general case the final expressions for the matrix elements of $\hat{R}$ are:

$$R_{\pm\pm} = \frac{1}{C}\left\{R_\pm \mp \frac{(k'^+ - k'^-)(k^+ + k^-)}{(k^- + k'^-)(k^+ + k'^+)}\sin^2(\chi/2)\right\}$$

$$R_{\pm\mp} = \frac{1}{C}\left\{-\frac{(k'^+ - k'^-)k^{\mp}}{(k^- + k'^-)(k^+ + k'^+)}\sin\chi\right\}$$

$$C = 1 - \frac{(k'^+ - k'^-)(k^- - k^+)}{(k^- + k'^-)(k^+ + k'^+)}\sin^2(\chi/2). \tag{5}$$

These formulas are useful to calculate the beam splitting, but the notations are not appropriate for an experiment, because both spin states in the incident beam are characterized by the same wave vector $\mathbf{k}^+ = \mathbf{k}^- = \mathbf{k}$ with a given normal component k. Thus, if we consider the splitting of the part of the beam initially polarized along the field, we must replace $k^2 - B_0$ by k^2 which means shifting of all k^2 in (5) by $+B_0$. Thus, k^+ for that part of the beam becomes $k^+ = \sqrt{k^2 + 2B_0}$, and $k'^{\pm} = \sqrt{k^2 - u + B_0 \pm B_1}$. For the part of the incident beam polarized in the opposite direction we must take $k^+ \equiv k$ and then $k^- = \sqrt{k^2 - 2B_0}$, and $k'^{\pm} = \sqrt{k^2 - u - B_0 \pm B_1}$.

It is easy to estimate the intensity of reflected beams in the case when the inside field is strong enough to make k'^- be imaginary, and leave k'^+ be real. In the first approximation with respect to B_0/k^2 the denominator can be replaced by 1 and the intensity of the off-specular beam becomes proportional to

$$|R_{-+}|^2 = k^2\left|\frac{-(k'^- - k'^+)}{(k^+ + k'^+)(k^- + k'^-)}\sin\chi\right|^2 = \frac{\gamma B_1 \sin^2\chi}{2(u + B_1)},$$

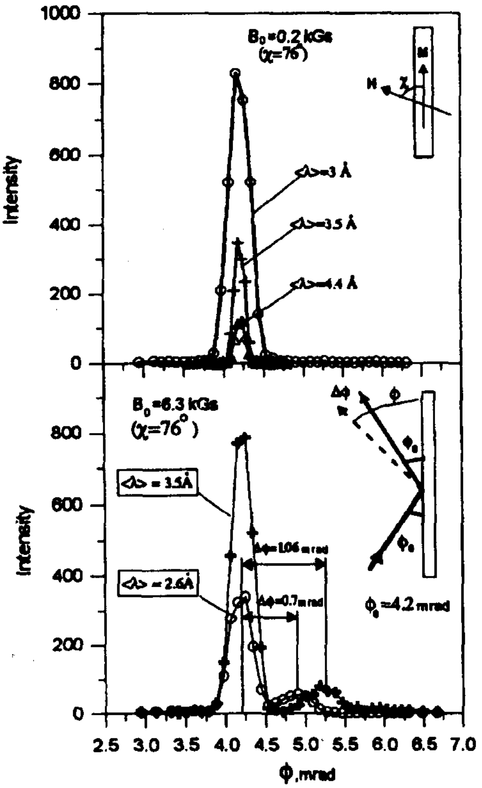
where $\gamma \approx |2k/(k + k'^+)|^2 \approx 1$.

Experiment. The experiment was performed with the time-of-flight reflectometer of polarized neutrons at the IBR-2 reactor in Dubna.

The sample was a thin anisotropic FeCo film on a glass substrate. The external field was applied either parallel to the anisotropy axis in the film plane ($\chi = 0$) or at an angle of 76 deg. to it (out of plane). The magnitude of the external field could be varied in the range $0.01 \div 7$ kGs. The polarized neutron beam with a wide Maxwellian spectrum was incident on the film at a grazing angle $\phi_0 = 4.2$ mrd. The polarization of the beam $P(\lambda)$ was a monotonous function decreasing from $P = 0.98$ at $\lambda = 1.8$ Åto $P = 0.5$ at $\lambda = 7$Å. The detector with a cadmium slit of 0.5 mm width was placed at 2.68 m from the sample. Thus, the angular aperture of the detector was $\delta\phi = 0.18$ mrd. To determine the reflection coefficients the intensity of the incident and reflected neutrons were measured at different orientations and magnitudes of the external field B.

For $\chi = 0$, the dependence of $N_+R_+ + N_-R_-$ on the wavelength was measured. Here, $N_\pm(\lambda)$ are proportional to the intensities of the incident neutrons with two spin projections on the external field, and $R_\pm$ are the squares of modules of the related reflection amplitudes.

For $\chi = 76$ deg., the angular distributions of the reflected neutrons were measured for two magnitudes of the external field: 0.2 and 6.3 kGs. (fig. 3).



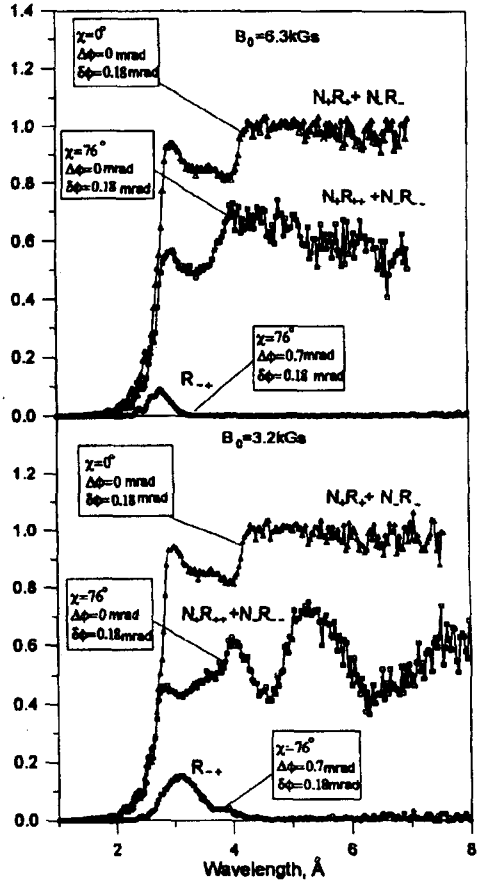


Fig.3. The dependence of the reflected neutron intensity on the angle ϕ of detector positioning. a) $B = 0.2$kGs, $\chi = 76°$, the detector aperture $\delta\phi = 0.18$ mrd, the grazing angle of the incident beam is $\phi_0 = 4.2$ mrd. The intensity distribution maximums for different λ are observed at the same specular angle $\phi = \phi_0$. b) $B = 6.3$kGs, $\chi = 76°$, $\delta\phi = 0.18$ mrd, $\phi_0 = 4.2$ mrd. The angular distribution of the reflected intensity for two different intervals of λ. In the vicinity of the specular beam ($\phi = \phi_0$), off-specular ones appear. The angular shift $\Delta\phi - \phi - \phi_0$ has the quadratic dependence on the averaged wavelength $< \lambda >$

Fig.4 The wavelength dependence of $N_+R_+ + N_-R_-$ in the specular direction $\phi = \phi_0$ for $\chi = 0$ and $\chi = 76°$ and of $|R_{-+}|^2$ for $\chi = 76°$ in the off-specular direction ($\Delta\phi = 0.7$ mrd.). a) $B = 6.3$ kGs, b) $B = 3.2$ kGs

In the field B=6.3 kGs, off-specular neutrons were observed at $\phi > \phi_0$. To determine the dependence of $\Delta\phi = \phi - \phi_0$ on λ the energy range of the counted neutrons was restricted to two intervals $\Delta\lambda_1$ and $\Delta\lambda_2$ around $\lambda_1 = 2.6$ and $\lambda_2 = 3.5$ Å, respectively. The measured ratio of the magnitudes $\Delta\phi_1(\lambda_1)$ and $\Delta\phi_2(\lambda_2)$ (fig 3b), satisfies the relation $\Delta\phi_1(\lambda_1)/\Delta\phi_2(\lambda_2) = (\lambda_1/\lambda_2)^2$ with the precision better than

0.5%, and corroborates the quadratic dependence of $\Delta\phi$ on λ. The measurements of $\Delta\phi$ at fixed λ and different B corroborate the linear dependence $\Delta\phi \propto B$.

For the fixed position of the detector at $\Delta\phi = 0.7$ mrd and two magnitudes of the external field: $B = 6.3$ and 3.2 kGs the spectral dependence of the square modules of R_{++}, R_{+-} and R_{-+} were measured (fig. 4). The spectral interval of the measurements was determined by the angular detector aperture $\delta\phi = 0.18$ mrd.

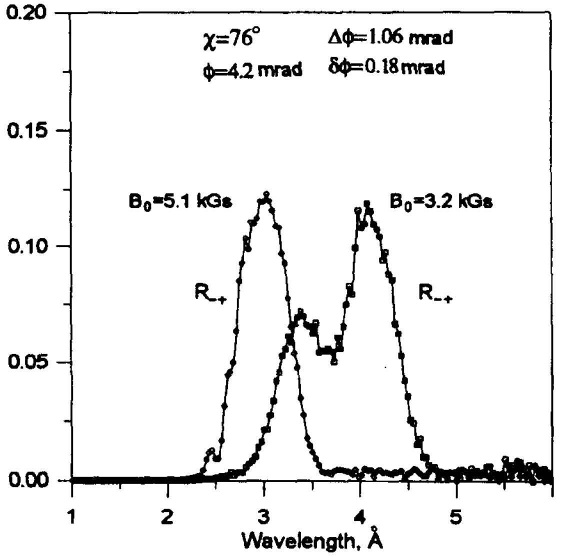


Fig.5. The dependence of $|R_{-+}|^2$ on λ for $\Delta\phi = 1.06$ mrd and two fields: $B = 5.1$ kGs, and $B = 3.2$kGs. The shift and broadening of the spectral interval for the weaker field corroborate the dependence $\Delta\phi \propto B\lambda^2$. The bell shaped forms of both spectra are related to the small aperture $\delta\phi = 0.18$ mrd of the detector

The probabilities $|R_{\pm\mp}(\lambda)|^2$ were also measured at $\Delta\phi = 1.06$ mrd for two magnitudes of the external magnetic field (fig. 5). The positions and spectral widths of the functions $|R_{\pm\mp}(\lambda)|^2$ corroborate the expected theoretical dependence $\Delta\phi \propto B\lambda^2$. It is evident that the measurement of the nondiagonal elements $|R_{\pm\mp}(\lambda)|^2$ in a wide spectral interval of λ in the off-specular direction requires detectors with a wide angular aperture contrarily to the measurement of the sum $N_+R_+(\lambda) + N_-R_-(\lambda)$ in the specular direction.

The obtained experimental data demonstrate that the relectometry in high external fields ($B \geq 2$ kGs) from noncollinear structures with nondiagonal reflection matrices reveals strong angular dispersion of the reflected neutrons with reversed spins. For the case of a nonpolarized incident beam the observation of this dispersion gives the opportunity to measure the nondiagonal elements $|R_{\mp\pm}(\lambda)|^2$ in the off-specular beams and the sum $N_+R_+(\lambda) + N_-R_-(\lambda)$ in the specular one. It also gives the opportunity to get information on the distribution of magnetization in films using nonpolarized neutrons.

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