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

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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 reflection angle. The particular case of reflection from a magnetic mirror with magnetization noncollinear to the external field is considered. The probability of spin reverse and a deviation of reflection angles from the specular one are calculated. The experiment to observe this effect is described and its results are reported.

The investigation has been performed at the Laboratory of Neutron Physics, JINR.

Незеркальное отражение нейтронов от магнитных сред
с недиагональными матрицами отражения

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Отражение нейтронов от магнитных сред описывается матрицей отражения с отличными от нуля, в общем случае, недиагональными компонентами, которые определяют вероятность переворота спина. Во внешнем поле переворот спина приводит к изменению кинетической энергии нейтрона и угла отражения. В работе рассматривается частный случай отражения от магнитного зеркала, намагниченность которого непараллельна внешнему полю. Вычисляется вероятность переворота спина и величина отклонения угла отражения от зеркального. Дано описание эксперимента и его результатов по наблюдению данного эффекта.

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1. 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 multiayered systems [2—6]. It was pointed out [7—13] that reflection from films with noncollinear magnetic structures is more complicated than reflection from films with collinear ones. In noncollinear case the reflection is characterized by the reflection matrix:

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

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

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 the off-specular reflection is described.

2. 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 [7,9]. 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 intensities of the side lobes are determined by the matrix elements R_{+-} and
R_{-+} of the matrix $\hat{R}$ and by 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 $\mathbf{k} = (\mathbf{k}_\|, \mathbf{k}_\perp)$ the wave vector of the incident neutron with the $\mathbf{k}_\perp$, $\mathbf{k}_\|$
being its normal and parallel to the surface components. In the external field $\mathbf{B}$ the neutron
has the potential energy $-\sigma \mathbf{B}$, where $\mathbf{B}$ is measured in $h^2/2m\mu$ (m, μ are the neutron mass
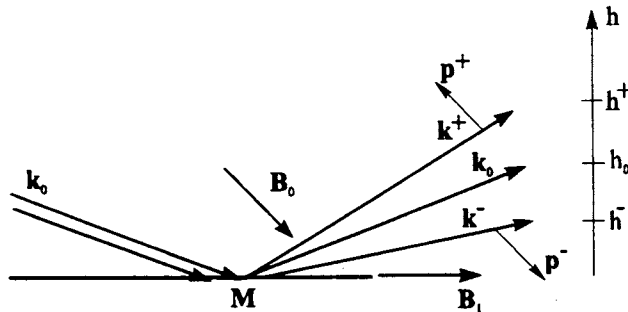

Fig.1. Following the reflection from a magnetized mirror with the
magnetization $\mathbf{M}$ noncollinear to the external magnetic field $\mathbf{B}_0$
the nonpolarized incident neutron beam with a wave vector k_0
splits into three beams. Two off-specular beams with the wave
vectors k^+ and k^- are ideally 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

Fig.2. The relative angular splitting of spin reversed beams in dependence on λ (in Angstroms) and the external magnetic field for $\phi_0 = 4.2$ mrd. The crosses are the experimental points (see Sec.4)
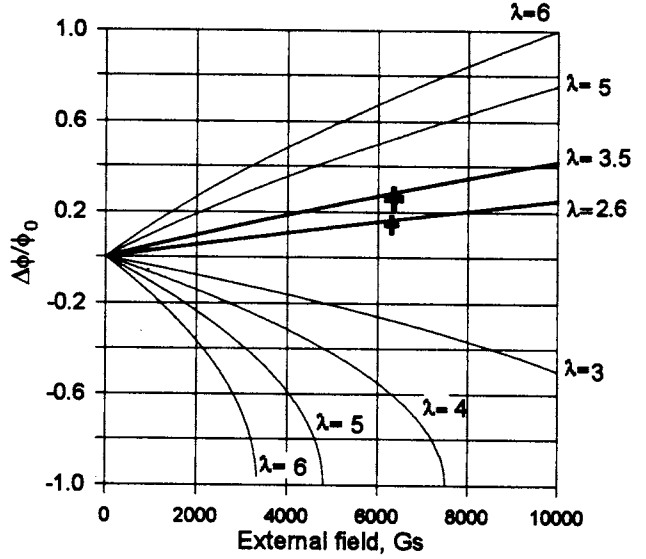
and magnetic moment, respectively) and σ are the Pauli matrices. On spin reverse the potential energy changes in magnitude by $\pm 2B$. Because of energy conservation it changes the kinetic energy: $k^2 \to k^2 \pm 2B$. In the reflection from an interface the components $\mathbf{k}_{\parallel}$, are also conserved. Thus the change of the kinetic energy means the change in the normal component $\mathbf{k}_{\perp}$: $k_{\perp} \to k_{\perp}^{\pm} = \sqrt{k_{\perp}^2 \pm 2B}$, and as a result leads to change in the reflection angle. It is not difficult to calculate the angular deviation of shifted beams. For a small grazing angle $\phi_0 = 10^{-2} + 10^{-3}$ we have

$$\frac{\Delta\phi^{\pm}}{\phi_0} = \frac{\Delta k_{\perp}^{\pm}}{k_{\perp}} = \sqrt{1 \pm 2B/k_{\perp}^2} - 1 = \sqrt{1 \pm 1.47 \cdot 10^{-10} B_0 \lambda^2/\phi_0^2} - 1.$$

Here the neutron wavelength λ is measured in Angstroms; B, in Gauss; and ϕ_0, in radians. The dependence of 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 $\Delta\phi < 0$.

3. 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:

$$(\Delta - u\theta(z > 0) + \sigma B(z) + k^2)\ \psi = 0, \tag{3.1}$$

where u is an optical potential of the mirror, which is supposed to fill the half space $z > 0$, θ is a 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 case when $\mathbf{B}_0$ is unparallel to $\mathbf{B}_1$. The solution is: $\psi(\mathbf{r}) = \exp(i\mathbf{k}_\parallel \mathbf{r}_\parallel)\, \xi(z)$, where

$$\xi(z) = \theta(z < 0)\,[\exp(i\hat{k}_\perp^+ z)\,\xi_0 + [\exp(-i\hat{k}_\perp^+ z)\,\hat{R}\xi_0] +$$

$$+ \theta(z < 0)\exp(i\hat{k}_\perp'^+ z)\,\hat{T}\xi_0, \qquad (3.2)$$

$\hat{R}, \hat{T}$ are reflection and transmission matrices, $\hat{k}_\perp^\pm = \sqrt{k_\perp^2 \pm \sigma B}$, $\hat{k}_\perp'^\pm = \sqrt{k_\perp^2 - u \pm \sigma B}$, 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 $\hat{T}$:

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

The solution of these equations can be represented as follows:

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

Here we shall consider in detail the matrix $\hat{R}$ only:

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

$$\hat{R} = (\hat{k}^- + \hat{k}'^-)(\hat{k}^+ - \hat{k}'^+)/N \equiv \hat{A}/N, \qquad (3.3)$$

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

$$N = \langle + \mid k^+k^- + \hat{k}'^+ \hat{k}'^- + \hat{k}'^-k^+ + k^-\hat{k}'^+\mid + \rangle,$$

where $\mid \pm \rangle$ represent the eigen states of the matrix σB_0: $\int B_0\mid \pm \rangle = \pm B_0\mid \pm \rangle$. Evaluation gives

$$N = (k^+ + k'^+)\,(k^- + k'^-) - (k'^- - k'^+)\,(k^+ - k^-)\,\sin^2(\chi/2), \qquad (3.4)$$

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 vectors $\mathbf{B}_0$ and $\mathbf{B}_1$. The numerator of (3.2) can be reduced to the form:

$$\hat{A} = k^-k^+ - k'^-k'^+ + \hat{k}^-\hat{k}'^+ - \hat{k}'^-\hat{k}'^+ =$$

$$= k^+k^- - k'^+k'^- + (1/2)\,(k'^- + k'^+)(\hat{k}^+ - \hat{k}^-) - (1/2)\,(k'^+ - k'^-)(\hat{k}^-\sigma b_1 + \sigma b_1\hat{k}^+),$$

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 are to calculate matrix elements of $\hat{A}$

$$\langle \pm \mid \hat{A}\mid \pm \rangle = (k^- \pm k'^-)(k^+ \mp k'^+) \pm (k'^+ - k'^-)(k^+ + k^-)\,\sin^2(\chi/2),$$

$$\langle \mp |\hat{A}| \pm \rangle = - (k'^{+} - k'^{-}) \, k^{\pm} \sin \chi.$$

In the case of $\chi = 0$ (and similarly for $\chi = \pi$) the matrix $\hat{R}$ becomes diagonal with the elements:

$$R_{+} = (k^{+} - k'^{+})/(k^{+} + k'^{+}), \quad R_{-} = (k^{-} - k'^{-})/(k^{-} + k'^{-}).$$

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

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

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

$$C = 1 - \frac{(k'^{+} - k'^{-}) \, (k^{-} - k^{+})}{(k^{-} + k'^{-}) \, (k^{+} + k'^{+})} \sin^2 (\chi/2). \tag{3.5}$$

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 (3.5) by $+ B_0$. Thus, $\mathbf{k}^{+}$ for that part of the beam becomes, $k^{+} = \sqrt{k^2 + 2B_0}$, and $k'^{\pm} = \sqrt{k^2 - u \pm (B_1 \pm B_0)}$. 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 $k'^{\pm} = \sqrt{k^2 - u \pm (B_1 \mp B_0)}$.

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'^{+} to 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 become proportional to

$$|R_{-+}|^2 = k^2 \left| \frac{- (k'^{-} - k'^{+})}{(k^{+} + k'^{+}) \, (k^{-} + k'^{-})} \sin \chi \right|^2 = \frac{\gamma B_1 \sin^2 \chi}{2(u + B_1)}, \quad \text{where } \gamma = |2k/(k + k'^{+})|^2 \approx 1.$$

4. Experiment

The experiment was performed at 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
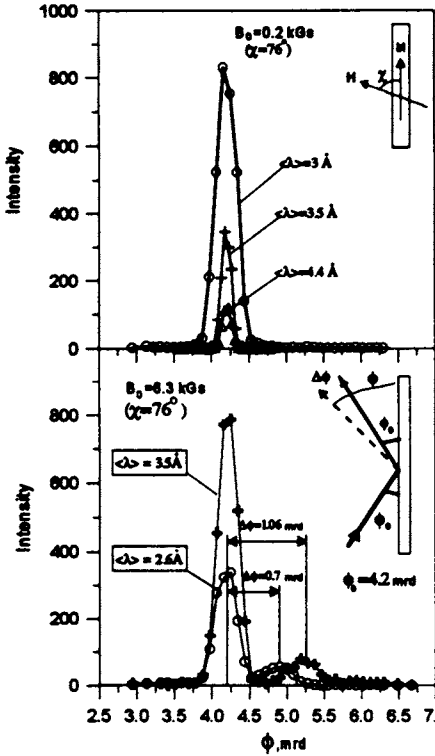
Fig.3. The dependence of the reflected neutron intensity on the angle ϕ of detector positioning. a) $B = 0.2$ kGs, $\chi = 76°$, the detector aperture $\delta\phi = 0.18$ mrd, the grazing angle of the incident beam is $\phi_0 = 4.2$ mrd. The intensity distribution maxima for different λ are observed 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 averaged wavelength $\langle \lambda \rangle$
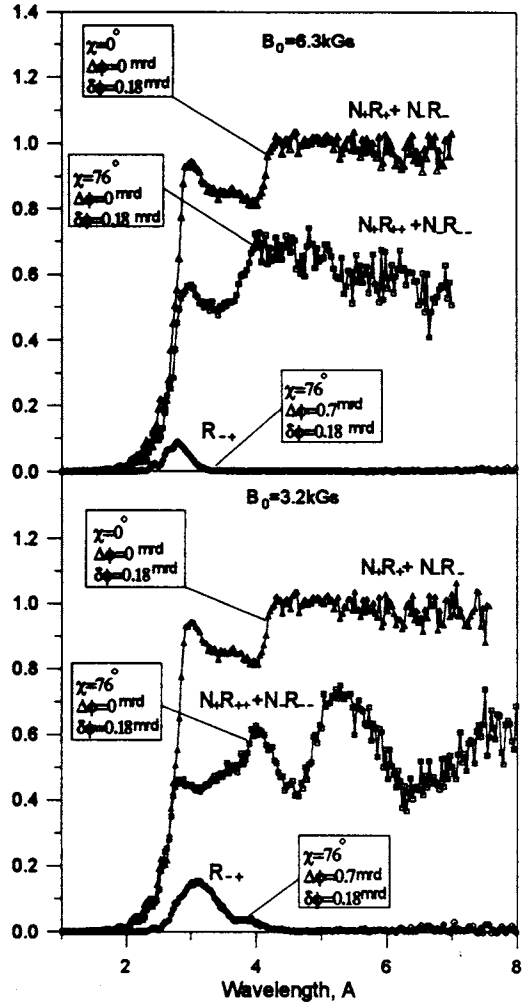
Fig.4. The wavelength dependence of $N_+R_+ + N_-R_-$ in the specular direction $\phi = \phi_0$ for $\chi = 0$ and $\chi = 76$ deg and of $|R_{-+}|^2$ for $\chi = 76$ deg in the off-specular direction ($\Delta\phi = 0.7$ mrd.). a) $B = 6.3$ kGs, b) $B = 3.2$ kGs

0.01 + 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 $\lambda = 1.8$Å to $P = 0.5$ 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 co-efficients the intensities of the incident and reflected neutrons were measured at different orientation 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). In the field $H = 6.3$ kGs, off-specular neutrons were observed at $\phi > \phi_0$. To determine the dependence of $\Delta\phi = \phi - \phi_0$ on lambda the energy range of counted neutrons was restricted to two intervals $\Delta\lambda_1$ and $\Delta\lambda_2$ around $\lambda_1 = 2.6$Å 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 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 $\phi = 0.18$ mrd. 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 position and spectral width of the functions $R_{\pm\mp}(\lambda)$ corroborate the expected theoretical dependence $\Delta\phi \propto B\lambda^2$. It is evident that measurement of nondiagonal elements
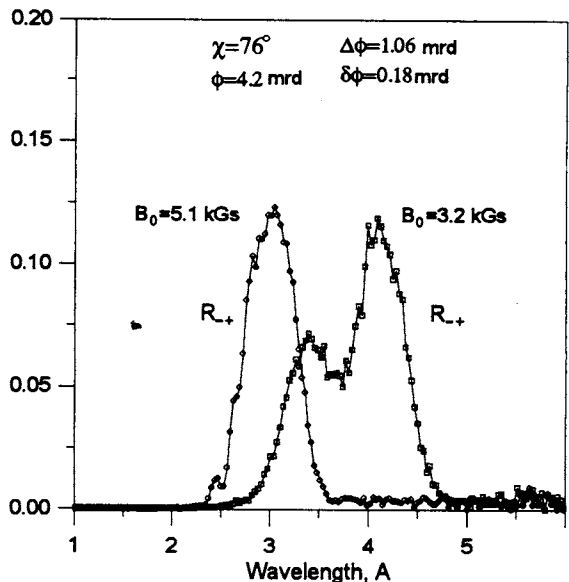

Fig.5. The dependence of $|R_+|^2$ on λ for $\Delta\phi = 1.06$ mrd and two fields: $B = 5.1$ kGs, and $B = 3.2$ kGs. The shift and broadening of the spectral interval for the weaker field corroborate the dependence $\Delta\phi \propto B\lambda^2$. The bell shaped forms of both spectra are related to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

$|R_{\pm\mp}(\lambda)|^2$ in a wide spectral interval of λ and in the off-specular direction requires detector with wide angular aperture contrary to the measurement of the sum $N_+R_{++}(\lambda) +$ $+ N_-R_{--}(\lambda)$ in the specular direction.

5. Conclusion

The obtained experimental data demonstrate that the reflectometry in high external fields ($B > 2$ kGs) from noncollinear structures with nondiagonal reflection matrices reveals strong angular dispersion of the reflected neutrons with reversed spins. For the case of nonpolarized incident beam the observation of this dispersion gives the opportunity to measure the nondiagonal elements $R_{\pm\mp}(\lambda)$ in the off-specular beams and the sum $1/2(R_{++}(\lambda) + R_{--}(\lambda))$ in the specular one. It also gives the opportunity to get information on the distribution of magnetization in films using nonpolarized neutrons.

References

1. Hughes D.J., Burgy M.T. — Phys. Rev., 1951, v.81, p.498.
2. Felcher G.P., Hildeke R.O., Crawford R., Haumann J., Kleb R., Ostrowski G. — Rev. Sci. Instr., 1987, v.58, p.609.
3. Korneev D.A., Pasyuk V.V., Petrenko A.V., Dokukin E.B. — Neutron Refectivity Studies on Superconducting, Magnetic and Absorbing Thin Films on the Polarized Neutron Spectrometer at the Pulsed Reactor IBR-2, In: H.Zabel, I.K.Robinson (Eds.) Surface X-Ray Neutron Scattering (Proceedings of the 2nd Int. Conf., Bad Honnef, Germany, June 25—28, 1991, p.213.
4. Lauter H.J., Bland J.A.C., Bateson R.D., Jonson A.D. — Magnetic Properties of Ultra-thin Co/Ag Films Investigated by Polarized Neutron Reflection, Ibid, p.219.
5. Endoh Y. — In: Neutron Optics Devices and Applications, C.Majkrzak, J.Wood, Editors, Proc. SPIE 1738, 1992, p.224.
6. Fitzimmons M.R., Smith G.S., Pynn R., Nastasi M.A., Burkel E. — Physica B, 1994, v.198, p.169.
7. Ignatovich V.K. — Pis'ma ZhETP, 1978, v.28, p.311 (see Sov. JETP Lett.).
8. Korneev D.A. — Poverhnost', 1989, v.2, p.13 (in Russian).
9. Ignatovich V.K. — The Physics of Ultracold Neutrons, Clarendon Press, Oxford, 1990.
10. Majkrzak C.F. — Physica B, 1991, v.173, p.75.
11. Korneev D.A., Chernenko L.P. — In: Neutron Optics Devices and Applications, C.Majkrzak, J.Wood, Editors, Proc. SPIE 1738, 1992, p.468.
12. Zabel H. — Physica B, 1994, v.198, p.156.