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THEORY OF NEUTRON CHANNELING IN RESONANT LAYER OF MULTILAYER SYSTEMS

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1 Introduction

We consider here theoretically neutron channeling in a planar system like the one shown in fig. 1 (in more details it will be considered in the next section). This system consists of two layers on a substrate, and optical

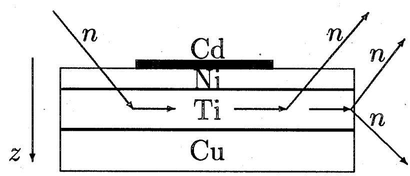

Figure 1: A mirror for measuring resonant neutron channeling.

potential of the system is shown in fig. 2 (without Cd). The channeling takes place in the second ("resonant") layer, which has low optical potential. In the figure it was supposed to be Ti, because Ti has a negative optical potential or potential well of depth u_2 (fig. 2). The substrate has a positive optical potential u_3. For example, it can be Cu, as shown in fig. 1. Substrate is usually thick enough for the waves channeled in Ti were totally reflected from it. Above Ti there is a "tunneling" layer. It also has a positive optical potential (u_1 in fig. 2) to hold channeled wave inside Ti. This potential can be even higher than that of the substrate ($u_1 > u_3$). For example, as shown in fig. 1, the tunneling layer can be Ni with potential higher than Cu. However it must be thin enough for the outside wave to penetrate (tunnel) into the resonant Ti layer. Atop the system there is shown a Cd layer, which absorbs neutrons, and prevents feeding of the channel along its length from outside.

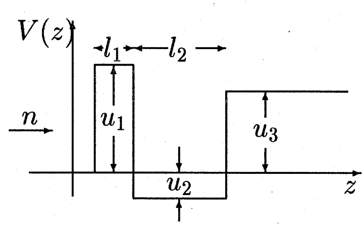

Figure 2: Stepwise potential of a multilayer resonant (MR) system. The z-axis is directed along normal to the surface of the multilayer system.

Such multilayer systems are well known (see for instance [1]), however there is no good understanding, how external wave is coupled to the channeling one. It is understood what happens, if the channel is a micro waveguide, in which the wave is an eigen mode. In this case the wave is totally reflected from both sides, and the waveguide is fed from outside through its entrance orifice at the edge surface or through a special wedge.

In our case the channel is not a perfect waveguide because its upper side is slightly permeable. So, instead eigen modes we have resonant ones, and the channel is fed just through the upper side. In this case we know well the wave function in the system under illuminated part of the upper surface (to the left of Cd in fig. 1), but we do not know, what is the channeling wave, how it propagates under nonilluminated area, and how it is matched at the interface between illuminated and nonilluminated parts. These are the main questions we address to in this paper.

The micro waveguides are well known for x-rays [2, 3, 4], where they are used for microfocusing, which is applied to microdiffraction, microimaging and microspectroscopy. Modern powerful synchrotron sources highly stimulated research in this field.

Neutron sources are considerably less powerful, and a single micro waveguide, if fed through the entrance, gives too low intensity because of too small area of the entrance hole. So it is interesting to look for the channeling in a geometry like the one shown in fig. 1.

First observation of neutron channeling [5] in thin films had shown that such experiments are feasible and worth of further theoretical and experimental consideration [6, 7, 8, 9, 10].

Experiments on neutron channeling in thin-film neutron wave guides were discussed in papers [11, 12, 13, 14, 15]. In the present letter we present some different approach. We show how to relate extinction of neutron flux along the channel with tunneling through the first layer, and how to find distribution of neutrons outgoing from the channel [11, 13].

The problems of channeling in MR systems are tightly related to the problems of reflection from them, which are studied by reflectometry. The resonant structure of the MR systems shows itself in interference pattern of reflectivity even at subcritical reflection, when normal to surface component E_z of the total energy of the incident beam is in the range $0 < E_z < u_3$. However this pattern has well pronounced resonant minima only when the system has high absorption in the middle layer.

Experiments on subcritical ($E_z < u_3$) reflection were reported in [16, 17, 18, 19, 20]. The depth of minima of reflectivity curve (dependence of reflectivity on neutron energy) was enhanced by special choice of material with high absorption for layer u_2, or by embedding a thin absorbing layer into the resonant one. Experiments were also performed with polarized neutrons and magnetic layers where spin rotation played the role of absorption.

In the next section we consider reflectivity of resonant systems and channeling in them.

2 Wave function in a multilayer system

We shall treat multilayers by method of multiple reflections presented in [21, 22, 23], which is applicable to scalar and magnetic systems. This method is analytical one, and it is more appropriate for our analysis than the other methods like [20, 24, 25], which, in our opinion, are more appropriate for numerical calculations.

We denote x the coordinate along the mirror and z the coordinate along normal to it. The wave function in the middle layer u_2 under area illuminated by the incident plane wave $\exp(ik_xx+ik_zz)$ is equal to

$$\psi(z,x)=A(k_z)[\exp(ik_{2z}z)+\exp(ik_{2z}l_2)\rho_{23}(k_{2z})\exp(-ik_{2z}(z-l_2)]\exp(ik_xx), \tag{1}$$

where $k_{2z}=\sqrt{k_z^2+u_2}$, k_z and k_x are the components of the neutron wave vector, and $\rho_{23}(k_{2z})$ is the reflection amplitude from the totally reflecting layer u_3 inside the layer u_2. The factor $A(k_z)$ is determined by the equation

$$A(k_z)=\tau_{12}+\rho_{21}\rho_{23}\exp(2ik_{2z}l_2)A(k_z), \tag{2}$$

which shows that the wave propagating toward the substrate is the sum of the wave penetrated through the tunneling layer from outside (the first term), and the wave reflected from the tunneling layer (the second term). The term τ_{12} is transmission amplitude through barrier u_1 from vacuum into the layer u_2, and ρ_{21} is reflection amplitude in the layer u_2 from the barrier u_1. From (2) it follows

$$A(k_z)=\frac{\tau_{12}}{1-\rho_{21}\rho_{23}\exp(2ik_{2z}l_2)}. \tag{3}$$

2.1 Neutron resonances in MR systems

Since reflection from u_3 is total, the amplitude ρ_{23} is of the form $\rho_{23}=\exp(i\phi_{23})$. After substitution of this ρ_{23} and $\rho_{21}=|\rho_{21}|\exp(i\phi_{21})$ into (1) the denominator becomes

$$1-\rho_{21}\rho_{23}\exp(2ik_{2z}l_2)=1-|\rho_{21}|\exp(2ik_{2z}l_2+i\phi_{23}+i\phi_{21}). \tag{4}$$

It has minima at points k_z, which satisfy the equation

$$2k_{2z}l_2+\phi_{23}(k_{2z})+\phi_{21}(k_{2z})=2\pi n \tag{5}$$

with integer n. At these points, which correspond to resonances, the amplitude $A(k_z)$ of the wave function (1) has maxima. The magnitudes of the maxima are larger the closer is $|\rho_{21}|$ to unity, or the smaller is transmission amplitude $|\tau_{21}|$.

Let us see how large are these maxima. If we neglect the losses we have the law of energy or flux conservation, which is the same as unitarity condition represented by the relation

$$k_{2z}|\rho_{21}|^2 + |\tau_{21}|^2 k_z = k_{2z}, \tag{6}$$

where τ_{21} is transmission amplitude through barrier u_1 out the layer u_2, and k_z, k_{2z} are normal to MR components of the neutron wave vector in vacuum and inside the u_2-layer. The relation (6) leads to

$$|\rho_{21}|^2 = \sqrt{1 - |\tau_{21}|^2 \frac{k_z}{k_{2z}}} \approx 1 - \frac{1}{2}|\tau_{21}|^2 \frac{k_z}{k_{2z}}, \tag{7}$$

for $|\tau_{21} \ll 1$.

From detailed balance theorem it follows that probability of transmission from vacuum into u_2-layer, and backward are equal. It gives

$$|\tau_{12}|^2 k_{2z}/k_z = |\tau_{21}|^2 k_z/k_{2z}. \tag{8}$$

This leads to $\tau_{21} = (k_{2z}/k_z)\tau_{12}$. Substitution into (7) and into (3) with account of (5) gives

$$|A(k_z)| = \frac{|\tau_{12}|}{1 - |\rho_{21}|} \approx \frac{2}{|\tau_{21}|} \gg 1. \tag{9}$$

For $|\tau_{21}| \approx 0.1$ we have at resonance $|A(k_z)|^2 \approx 400$.

2.2 Mechanism of particle accumulation in the resonant layer

We can easily understand the mechanism of wave function enhancement at resonances in the u_2-layer. Indeed, at resonances the wave

$$\exp(ik_{2z}l_2)\rho_{23}(k_z)\exp(-ik_{2z}[z - l_2])$$

in (1) going from substrate toward u_1-layer after reflection at the point $z = 0$ becomes equal to

$$\exp(2ik_{2z}l_2)\rho_{23}(k_z)\rho_{21}(k_z)\exp(ik_{2z}z) = |\rho_{21}|\exp(ik_{2z}z)$$

because of (5), i.e. it positively interferes with previous wave $\exp(ik_{2z}z)$ and enhances it.

Such enhancement facilitates penetration of the external wave into u_2-layer. It means that reflection amplitude of the external wave decreases, and we want to prove that this is indeed so.

Let us consider the resulting amplitude of the outgoing wave consisting of two parts: the directly reflected incident wave with amplitude ρ_{12} and the one, which is transmitted into u_2 layer, then reflected from substrate and transmitted back into vacuum. The amplitude of the second wave is equal to $\tau_{12}\tau_{21}\rho_{23}(k_z)\exp(2ik_{2z}l_2)$. Thus resulting reflection amplitude is

$$\tilde{\rho}_{12} = \rho_{12} + \tau_{12}\tau_{21}\rho_{23}(k_z)\exp(2ik_{2z}l_2) = \rho_{12}\left[1 + \frac{\tau_{21}\tau_{12}}{\rho_{21}\rho_{12}}|\rho_{21}|\right], \tag{10}$$

where in the last equality we took into account (5). It is easy to show [22, 26] that

$$\rho_{12} = \frac{r_{01} - r_{21}\exp(-2k_{1z}l_1)}{1 - r_{01}r_{21}\exp(-2k_{1z}l_1)}, \qquad \rho_{21} = \frac{r_{21} - r_{01}\exp(-2k_{1z}l_1)}{1 - r_{01}r_{21}\exp(-2k_{1z}l_1)}, \tag{11}$$

$$\tau_{12} = \frac{t_{01}t_{12}\exp(-k_{1z}l_1)}{1 - r_{01}r_{21}\exp(-2k_{1z}l_1)}, \qquad \tau_{21} = \frac{t_{21}t_{10}\exp(-k_{1z}l_1)}{1 - r_{01}r_{21}\exp(-2k_{1z}l_1)}, \tag{12}$$

$$r_{01} = \frac{k_z - ik_{1z}}{k_z + ik_{1z}}, \qquad r_{21} = \frac{k_{2z} - ik_{1z}}{k_{2z} + ik_{1z}}, \qquad k_{1z} = \sqrt{u_1 - k_z^2},$$

$$t_{01} = \frac{2k_z}{k_z + ik_{1z}}, \qquad t_{21} = \frac{2k_{2z}}{k_{2z} + ik_{1z}}, \qquad t_{10} = \frac{2ik_{1z}}{k_z + ik_{1z}}, \qquad t_{12} = \frac{2ik_{1z}}{k_{2z} + ik_{1z}}, \tag{13}$$

where r_{ik} denotes reflection and t_{ik} transmission amplitudes for a potential step from level u_i to level u_k, and l_1 is the width of the u_1-layer.

For real potentials u_1, u_2 we have $\tau_{21}\tau_{12}/\rho_{21}\rho_{12} = -|\tau_{21}\tau_{12}|/|\rho_{21}\rho_{12}|$. Substitution into (10) gives

$$\tilde{\rho}_{21} = \rho_{12}\left[1 - \frac{|\tau_{12}\tau_{21}|}{|\rho_{12}\rho_{21}|}|\rho_{21}|\right], \tag{14}$$

or $|\tilde{\rho}_{12}| < |\rho_{12}|$. It shows that indeed the wave passed through the resonance layer compensates a little bit the directly reflected one.

However at energies $E_z < u_3$ reflection is always total independently of the E_z, thus the amplitude in the resonant layer should be accumulated to such a level that the wave transmitted through u_1 into vacuum would overcompensate the directly reflected one and bring the module of the resulting reflected amplitude to unity. Indeed, if we multiply the second term in the brackets of expression (14) by the resonant factor $1/(1-|\rho_{21})$, we obtain

$$\rho_r = \rho_{12}\left[1 - \left|\frac{\tau_{21}\tau_{12}}{\rho_{21}\rho_{12}}\right|\frac{|\rho_{21}|}{1-|\rho_{21}|}\right] =$$

$$\frac{\rho_{12}}{|\rho_{12}\rho_{21}|}\frac{|\rho_{12}\rho_{21}| - |\rho_{21}|(|\rho_{12}\rho_{21}| + |\tau_{12}\tau_{21}|)}{1-|\rho_{21}|} = -\frac{\rho_{12}}{|\rho_{12}|}, \qquad (15)$$

where we used relations

$$|\rho_{12}\rho_{21}| + |\tau_{12}\tau_{21}| = 1,$$

and $|\rho_{12}| = |\rho_{21}|$, which directly follow from (11,12). Expression (13) shows that the resulting reflection is indeed total.

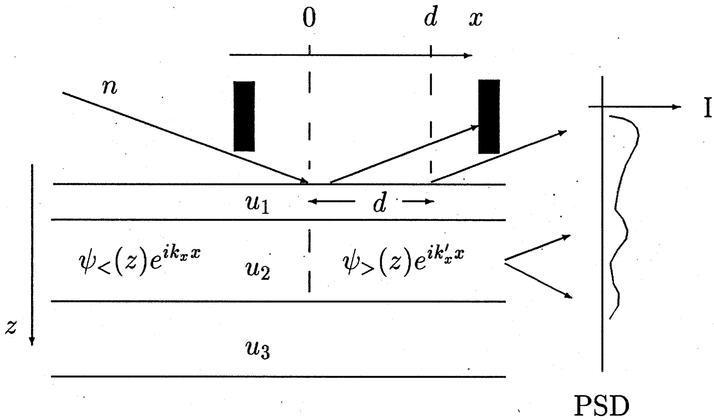

Figure 3: Matching the wave function at $x = 0$ in two parts of a multilayer mirror, and distribution of outgoing neutrons over position sensitive detector PSD.

2.3 Channeling in the middle layer

To start discussion of our ideas for the channeling let us consider a system slightly different from that one shown in fig. 1. It will be easier for us, if illumination is stopped by absorbers arranged as shown in fig. 3. It is easier because boundary conditions under nonilluminated area remain the same as under illuminated one, which means that resonant conditions remain the same. In the case of fig. 1 reflectivity in resonant layer from upper side under nonilluminated area is different from that under illuminated one, and positions of resonances should be slightly shifted. It leads to some complication for matching at interface between illuminated and nonilluminated parts. In our geometry the front of the incident wave is limited by an absorber, and the position sensitive detector (PSD) does not see the illuminated part of the mirror.

Under illuminated part of the mirror ($x < 0$) the wave function inside the layer u_2 is equal to

$$\psi_<(x,z) = A(k_z)[e^{ik_{2z}z} + e^{ik_{2z}l_2}\rho_{23}(k_{2z})e^{-ik_{2z}(z-l_2)}]\exp(ik_x x), \qquad (16)$$

where k_x is the component along x-axis of the wave vector in the incident wave above the mirror, and the coefficients A, ρ_{23}, and wave number k_{2z} are the same as in (1).

The wave function under nonilluminated surface is a solution of the Schrödinger equation, which we can represent in the form:

$$\psi_>(x,z) = A[\exp(ik'_{2z}z) + \exp(ik'_{2z}l_2)\rho_{23}(k'_{2z})\exp(-ik'_{2z}(z-l_2))]\exp(ik'_x x), \qquad (17)$$

where $A = A(k_z)$, and $k'^2_{2z} + k'^2_x = k^2 + u_2$. If we take $k'_{2z} = k_{2z} - i\kappa$, where $k_{2z} = \sqrt{k_z^2 + u_2}$, then $k'_x = \sqrt{k_x^2 + 2i\kappa k_{2z}} \approx k_x + i\kappa k_{2z}/k_x$, where $k_x^2 = k^2 - k_z^2$. The imaginary part, $\kappa > 0$, should be chosen in such a way that

$$\rho_{21}(k'_{2z})\rho_{23}(k'_{2z})\exp(2ik'_{2z}l_2) = 1. \qquad (18)$$

This form matches well the wave function (17) to the right and (16) to the left of section $x = 0$. Some mismatch because of κ gives some reflected wave going to the left from section $x = 0$. However for small κ, and we shall soon see, when it is small, the reflected wave is also small, so we shall neglect it for now.

The equation (18) is the same as (2) but with τ_{12} omitted. When it is satisfied, the wave function has the same dependence on z at every point x, and only its amplitude $|A|$ contains a factor, which, because of imaginary part of k'_x, exponentially decays along x-axis:

$$\exp(ik'_x x) = \exp(ik_x x)\exp\left(-\frac{x}{2x_e}\right), \quad \frac{1}{2x_e} = \kappa\frac{k_{2z}}{k_x}. \qquad (19)$$

In the case when $|\rho_{21}| - 1 \ll 1$ the magnitude of κ is small and we can neglect it in amplitudes ρ_{23} and ρ_{21}. Then (18) is represented as:

$$|\rho_{21}(k_z)|\exp(2ik_{2z}l_2 + i\phi_{23} + i\phi_{21} + 2\kappa l_2) = 1. \qquad (20)$$

For k_{2z} satisfying condition (5) we obtain $|\rho_{21}|\exp(2\kappa l_2) = 1$, which gives the magnitude of κ:

$$\kappa = -\frac{1}{2l_2}\ln(|\rho_{21}(k_{2z})|) \approx \frac{k_z}{4l_2k_{2z}}|\tau_{21}(k_{2z})|^2 = \frac{k_{2z}}{4l_2k_z}|\tau_{12}(k_z)|^2, \qquad (21)$$

where relations (7,8) were taken into account. Thus $\kappa \ll k_{2z} \approx 2\pi/l_2$ when $|\tau_{12}|^2 \ll 8\pi k_{2z}/k_z$, which is always satisfied, so our approximation is always very well justified.

Let us estimate the range $x_e \equiv k_x/2k_{2z}\kappa = 2l_2 k_x/k_z|\tau_{21}|^2$ of exponentially decaying factor in (19). For neutrons with wavelength 4 Å, in particular, the grazing angle of incidence is small (we need total reflection from substrate), so $k_z/k_x \approx 10^{-3}$. Thus $x_e = 2 \cdot 10^3 l_2/|\tau_{21}|^2$. For $|\tau_{21}| \approx |\tau_{12}| \approx 0.1$ and $l_2 = 2000$ Å we have $x_e = 4$ cm.

2.4 Intensity distribution over nonilluminated surface

All the above formulas were obtained for a single incident neutron. Then its flux over unit area of entrance surface is proportional to k_z. For intensity I_0 we need to renormalize the coefficient A by factor $\sqrt{I_0/k}$. Then the number of neutrons crossing in a unit time the cross area of resonant layer at some point x under nonilluminated surface of the mirror is

$$J(x) = \frac{dN(x)}{dt} = \frac{I_0}{k}\int_0^{l_2} w dz |\psi(z)|^2 k_x \exp(-x/x_e), \qquad (22)$$

where w is the width of the mirror surface along y-axis.

From (17) it follows that

$$|\psi(z)|^2 \approx 4|A|^2 \cos^2(k_{2z}[z - l_2] - i\phi_{23}/2). \qquad (23)$$

Substitution into (22) gives integral

$$\int_0^{n\pi} \cos^2(\chi)d\chi = \frac{n\pi}{2}, \text{ where } \chi \approx k_{2z}z,$$

and n is the integer of the resonance $k_{2z}l_2 = n\pi$. Thus (22) is

$$J(x) = 2I_0\frac{k_x}{k}wl_2|A|^2 \exp(-x/x_e). \qquad (24)$$

From (24) it follows that the total number of neutrons crossing per unit time the section of the channel u_2 at the point $x = 0$ is

$$J(0) = 2I_0\frac{k_x}{k}wl_2|A|^2. \qquad (25)$$

At resonance, when (9) is valid, for $w = 1$ cm, $|A|^2 = 400$ and $l_2 = 2 \cdot 10^{-5}$ cm we have $J(0) \approx 10^{-2}I_0$.

Now we can calculate the total number of neutrons that go out through an element wdx of the nonilluminated surface at point x:

$$dJ(x) = -\frac{dJ(x)}{dx}dx = \frac{I_0}{k}wdx|A|^2|\tau_{21}|^2k_z\exp(-x/x_e) \equiv \frac{J(0)}{x_e}e^{-x/x_e}dx. \tag{26}$$

If nonilluminated area is infinite in x direction, then total number of outgoing neutrons is equal to the integral over dx from 0 to ∞, which is naturally is equal to $J(0)$.

The above result is valid for monochromatic and collimated neutrons with precisely resonant normal component k_z^2 of the neutron energy. If spectrum is not monochromatic, we should replace (25) with the expression

$$J(0) = 2\frac{dI_0(k_z^2)}{dk_z^2}\Gamma\frac{k_x}{k}wl_2|A|^2, \tag{27}$$

where Γ is the resonance width. This width is calculated as follows. Let us denote phase (5) as $\Phi(k_z)$, then the resonance condition (5) looks $\Phi(k_z) = 2\pi n$, where n is an integer ($n \geq 0$) called resonance order. Near n-th resonance the $\exp(i\Phi)$ in the denominator (4) can be approximated as

$$\exp(i\Phi) \approx 1 + i\frac{d\Phi}{dE}(E - E_n) \approx 1 + i\frac{l_2}{k_{2z}}(E - E_n), \tag{28}$$

where $E = k_z^2$. Substitution into (3) gives

$$A(k_z) = \frac{iC}{E - E_n + i\Gamma}, \tag{29}$$

where

$$\Gamma = \frac{k_{2z}}{l_2}\frac{1 - |\rho_{21}|}{|\rho_{21}|} \approx \frac{|\tau_{21}|^2k_z}{2l_2} \approx \frac{2k_z}{l_2|A|^2}, \qquad C = \tau_{12}\frac{k_{2z}}{l_2|\rho_{21}|}, \tag{30}$$

and we approximated $d\Phi/dE$ as $2l_2(dk_{2z}/dE) = l_2/k_{2z}$, because of weak dependence of phases ϕ_{23} and ϕ_{21} on energy.

Substitution of (30) and (9) into (27) gives

$$J(0) = 4\frac{dI_0(k_z^2)}{dk_z^2}wk_z. \tag{31}$$

For estimation we can replace $dI_0/dk_z^2 = I_0/k_z^2$, $k_z = \pi/l_2$, and accept $w = 1$ cm, $l_2 = 2 \cdot 10^{-5}$ cm, then we obtain

$$J(0) = 4I_0\frac{w}{k_z} \approx \frac{4}{\pi}I_0wl_2 \approx 2 \times 10^{-5}I_0, \tag{32}$$

which means that the experiment is feasible for $I_0 \propto 10^7$ n/sec/cm^2.

For distribution of exit neutrons over nonilluminated surface in experiment with geometry shown in fig. 3 we, according to (26), can expect the count rate

$$\frac{dJ(x)}{dx} = \frac{\Gamma}{k_z^2}\frac{J(0)}{x_e}e^{-x/x_e} \approx \frac{4}{\pi x_e} I_0 w l_2 e^{-x/x_e}, \tag{33}$$

and for above parameters we get

$$dJ/dx \approx 0.5 \times 10^{-5} I_0 \exp(-x/x_e)\frac{1}{\text{sec cm}}.$$

For the experiment with the geometry shown in fig. 1, we can get the similar estimation though matching under Cd is worth because of change of reflection amplitude $\rho_{21} \to \rho'_{21}$ at the upper surface of the layer u_2 and consequently some shift of the resonant value of k_{2z}. This matching will lead to excitation of several modes under Cd and reflection from the section at the point $x = 0$ to the left.

The above considerations can be generalized to the case, when absorbtion in the layers and scattering on inhomogenieties and interface roughnesses are not negligible. In that case all the formulas must be multiplied by the ratio

$$\frac{\Gamma^2}{(\Gamma + \Gamma_l)^2},$$

and the extinction length x_e should be changed to X_e, where

$$\frac{1}{X_e} = \frac{1}{x_e} + \frac{1}{x_l},$$

Γ_l and x_l describe losses because of absorbtion and scattering on roughnesses and inhomogenieties.

We can also easily generalize the above considerations to magnetic multilayer systems with noncollinear magnetization of nearby layers. See, for example, [23, 25].

3 Summary

We considered neutron channeling in a multilayer system. We applied to it simple analytical algebra, and we have shown how to match illuminated and nonilluminated areas in resonant layer. For matching we used the anzats (17), which represents wave function of channeled neutron under nonilluminated area. This wave function precisely satisfies Schrödinger equation in the resonant layer, is almost identical to the wave function on the other side of matching cross area, and determines the extinction rate of the channeling function along the channel in the absence of losses in the resonant layer. It is trivial to add losses, if they are present, and we leave it to a reader. Our estimations show that a neutron channeling experiment is feasible. For cold neutrons with nonmonochromatic intensity I_0 we can expect count rates of the order $10^{-5} I_0$, which are measurable in sufficiently good background conditions. For x-rays situation on one side is considerably better because of high luminosity of x-ray sources, but on the other side it is considerably worse because of high absorption of x-rays in matter. However these two factors can cancel each other and for x-rays we can expect the good feasibility too.

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Теория каналирования нейтронов
в резонансном слое многослойных систем

Представлена теория каналирования нейтронов в резонансных многослойных системах и рассмотрен эксперимент для проверки теории.

Работа выполнена в Лаборатории нейтронной физики им. И.М.Франка ОИЯИ.

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Theory of Neutron Channeling
in Resonant Layer of Multilayer Systems

A wave theory of neutron channeling in resonant multilayer systems is presented. An experiment to check the theory is considered.

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

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