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MONTE CARLO SIMULATION  
OF THE NONSTATIONARY TRANSPORT  
OF VERY COLD AND ULTRACOLD NEUTRONS  
IN VERTICAL NEUTRON GUIDES  
AND THE STORAGE OF ULTRACOLD NEUTRONS

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# 1 Introduction

In our previous article [1] we considered the nonstationary UCN transport in horizontal neutron guides. Sometimes the vertical arrangement of neutron guides for UCN extracting is more convenient or even possible in view of some peculiarities of reactor construction. In the vertical arrangement the energy of neutrons exiting from the moderator is higher than their energy during storage in experimental chamber.<sup>1</sup> It leads to better neutron transmission through membranes of the cooled moderator due to lower capture and scattering cross sections, and permits to use the most promising moderators for UCN production with high boundary energy, such as liquid [2] or solid deuterium [3], or deuterated methane. Both UCN sources currently in operation: ILL [4] and SPNPI (Gatchina) [5], have vertical neutron guides. On the other hand, however, the vertical arrangement of channels for UCN extracting leads to larger neutron losses due to larger probabilities of neutron diffuse scattering and capture at neutron reflection from the guide walls. In the vertical arrangement the VCN transport in the gravitational field has different spectral and time characteristics of neutron arrival distribution following a reactor pulse from the horizontal case. Difference in arrival time distributions leads to different from the horizontal case UCN storage characteristics important for the realization of the **non-stationary** UCN storage through neutron guides using a pulsed neutron source with pulses well separated in time [6]. Monte Carlo simulation of the nonstationary VCN and UCN transport in straight and curved vertical neutron guides with realistic surface roughness reveals some interesting features of transmission

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<sup>1</sup>The term UCN refers to neutrons stored in experimental chambers and having energies below the boundary energy of the chamber,  $E_b \sim 200 \text{ neV}$ ; VCN, starting from the moderator and then during transport decelerating to the UCN energy range, have greater energies.

of neutrons with different energies and of nonstationary storage and can be used to choose the best channel configuration.

## 2 Method of simulating the transport and storage of UCN

Five neutron guide configurations are shown in fig.1. These configurations were chosen for a prototype of the UCN source at the TRIGA type pulse reactor. All guides have rectangular cross sections ( $6 \times 6\text{cm}$ ).

In all calculations the primary VCN angular distribution has the form:

$$dw(\Omega) \sim \cos\theta \cdot d\Omega, \quad (1)$$

where  $\theta$  is the VCN momentum polar angle relative to an axis normal to the entrance window of the neutron guide.

The angular distribution of UCN elastically reflected from the guide internal surface is assumed to consist of two parts: specular and diffuse.

For the case of a surface with very low roughness the angular distribution of diffusively reflected neutrons was derived in [7], where the neutron momentum transfer dependence of the diffuse reflection probability had the form:

$$w_{d.r.}(\Omega_0, \Omega) = \frac{k_b^4}{4\cos\theta_0} \cdot |S(\theta_0)|^2 \cdot |S(\theta)|^2 \cdot F(\kappa), \quad (2)$$

for the diffuse neutron scattering away from the wall, and

$$w_{d.r.}(\Omega_0, \Omega) = \frac{k_b^4}{4\cos\theta_0} \frac{k'}{k} \cdot |S(\theta_0)|^2 \cdot |S'(\theta')|^2 \cdot F(\kappa),$$

$$\text{for } \cos^2(\theta') \cdot k'^2 > -k_b^2,$$

$$w_{d.r.}(\Omega_0, \Omega) = 0, \quad \text{for } \cos^2(\theta') \cdot k'^2 < -k_b^2, \quad (3)$$

for the diffuse neutron scattering into the wall.<sup>2</sup>

In these formulas:

$$S(\theta) = \frac{2\cos\theta}{\cos\theta + (\cos^2\theta - k_b^2/k^2)^{1/2}}, \quad (4)$$

$$S'(\theta') = \frac{2\cos\theta'}{\cos\theta' + (\cos^2\theta' + k_b^2/k'^2)^{1/2}}, \quad (5)$$

In these expressions  $k$  is the wave vector of incident (and reflected away from the wall) neutrons,  $k'$  is the wave vector of diffusively scattered neutron inside the wall characterized by the boundary wave vector  $k_b$ .

$$F(\kappa) = \sigma^2 T^2 / 2\pi \cdot \exp(-\kappa^2 T^2 / 2), \quad (6)$$

$$\kappa^2 = (\vec{k}_{\parallel} - \vec{k}_{\parallel 0})^2, \quad (7)$$

$\vec{k}_{\parallel 0}$  and  $\vec{k}_{\parallel}$  are the parallel to the surface plane components of incident and scattered wave vectors, so that

$$(\vec{k}_{\parallel} - \vec{k}_{\parallel 0})^2 = k^2(\sin^2\theta_0 + \sin^2\theta - 2\sin\theta \cdot \sin\theta_0 \cdot \cos(\phi - \phi_0)). \quad (8)$$

Here  $\theta_0$  and  $\theta$ ,  $\phi_0$  and  $\phi$  are the polar and azimuth angles of incident to the surface normal and reflected neutrons, respectively;  $\sigma$  and  $T$  in (6) are the surface roughness parameters for random deviations of the surface from the ideal plane geometry which are described by an autocorrelation function:

$$f(\vec{\rho} - \vec{\rho}') = \sigma^2 \cdot \exp(-(\vec{\rho} - \vec{\rho}')^2 / 2T^2). \quad (9)$$

The considered in our simulations surface roughness parameters  $\sigma = 30\text{\AA}$ ,  $T = 250\text{\AA}$  are quite realistic [7, 8, 11] for polished metal and glass surfaces with a metal coating.

<sup>2</sup>These restrictions, written here as they were done in eq.(21) of ref.[7] are not quite correct. We used in our simulations different restrictions:  $k'^2 > 0$  for upper eq.(3) and  $k'^2 < 0$  for the lower one.

UCN losses due to capture and inelastic scattering are described by the expression:

$$\mu(k, \theta) = 2\eta \frac{k \cdot \cos\theta}{k_b} \left/ \sqrt{1 - \left(\frac{k \cdot \cos\theta}{k_b}\right)^2} \right. \quad (10)$$

Here  $\theta$  is the incident angle to the surface normal, loss coefficient  $\eta = Im\ b/Re\ b$ ,  $Im\ b = (\sigma_c + \sigma_{in})/2\lambda$ ,  $\sigma_c$  and  $\sigma_{in}$  are the capture and the inelastic cross sections, respectively. In calculations we take  $\eta = 5 \cdot 10^{-4}$ . This value is approximately twice as large as the theoretical value of  $\eta$  for nickel or stainless steel.

Neutrons with energies higher than the boundary energy of the internal surface material of the guide have the possibility to penetrate the bulk material – **the main phenomenon with which the loss process works**. The neutron reflection probability in this case has the form:

$$R = \left| \left( k_{\perp} - \sqrt{k_{\perp}^2 - k_b^2} \right) / \left( k_{\perp} + \sqrt{k_{\perp}^2 - k_b^2} \right) \right|^2, \quad (11)$$

where  $k_{\perp}$  stands for the normal component of the neutron incident wave vector.

The boundary energy of the internal surface of all guides considered in these calculations is  $E_b = 207\text{neV}$ ,  $v_b = 6.3\text{m/s}$ , which corresponds to stainless steel properties – the most practical material.

In all calculations gravity, which bends neutron trajectories inside the guides, was rigorously taken into account.

Expressions (2) and (3) were used to describe the transmission of cold neutrons through a neutron guide in [8, 9] and of UCN in [10], and was simulated and experimentally verified [11] by the measurement of the transmission and angular distribution of cold neutrons emerging from straight neutron guides made of plexiglas and glass panes – both covered with  $0.2\mu\text{m}$  evaporated Ni.

To simulate UCN storage in experimental chambers of finite volume the outgoing VCN spectrum was assumed to be the normalized maxwellian spectrum in the interval of the starting velocities of neutrons which can be stored (in an infinite volume chamber) being channeled through ideal vertical neutron guide 7m height.

It is also assumed that the UCN life time in an experimental storage chamber at the end of the neutron guide (fig.1), can be written as:

$$\tau = 4V/sv, \quad (12)$$

where  $V$  is the volume of the storage chamber,  $s$  is the entrance window area and  $v$  is the neutron velocity. It is assumed that neutrons leaving the storage volume through the entrance window do not return to the chamber from the neutron guide. This simplification leads to some underestimation of the quantity of stored neutrons.

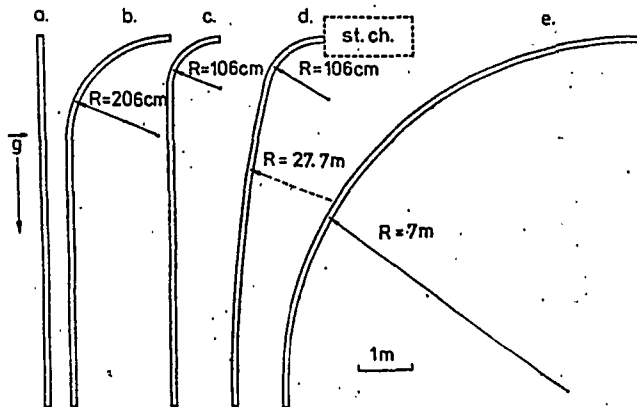


Fig.1 Neutron guides configurations used in Monte Carlo simulations. (st.ch. - storage chamber).

### 3 Results of the calculation

Some of the results of calculation are illustrated in figs.2-7. All calculations are based on at least 1,000 histories for each velocity (up to 10,000 histories for calculating arrival time and spectral distributions).

Figure 2 shows the VCN arrival velocity dependence of transmission through ideal guides. The characteristic slant on the transmission curve for curved vertical neutron guides at lower velocities (figs.2 and 4) is due to the return of very low velocity UCN in the gravitational field following their reflections from the guide walls in the curved top part of the guide (it does not take place in the horizontal neutron guides [1]). A decrease in transmission through curved guides at higher neutron velocities is the well known effect of in-wall losses of neutrons with veloci-

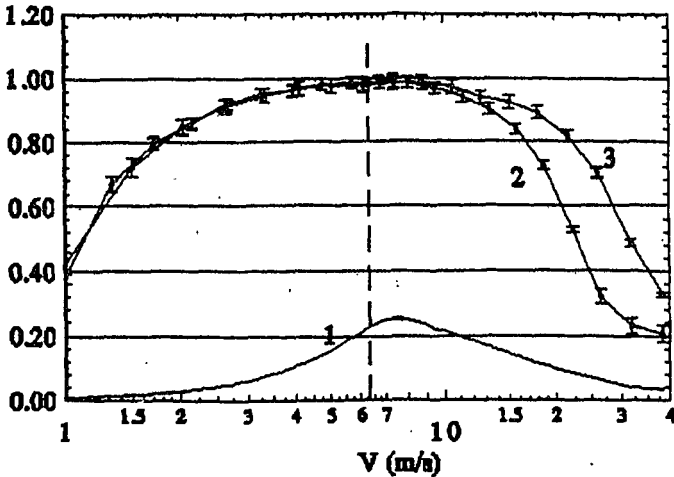


Fig.2 The arrival velocity dependence of neutron transmission through ideal vertical guides (in the absence of neutron capture and surface roughness): 1) configuration "a" from fig.1, curve is normalized to one neutron, corresponding to the indicated arrival velocity, incoming at the guide entrance with the angular distribution according to eq.(1); 2) configurations "c" and "d"; 3) configuration "b"; the upper curves are normalized to transmission through a straight guide of configuration "a".

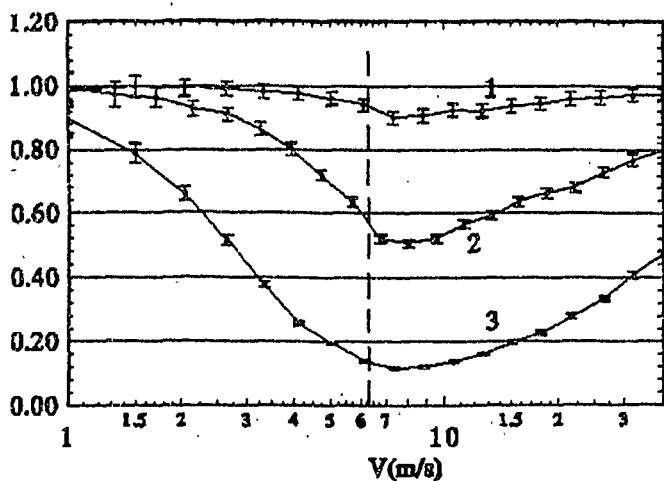


Fig.3 The arrival velocity dependence of neutron transmission through the **straight** guide in fig.1(a): 1) capture coefficient  $\eta = 5 \cdot 10^{-4}$ ; 2)  $\eta = 5 \cdot 10^{-3}$ ; 3)  $\eta = 5 \cdot 10^{-4}$ , surface roughness parameters  $\sigma = 30 \text{ \AA}$ ,  $T = 250 \text{ \AA}$ . All curves are normalized to transmission through ideal straight vertical guide of fig.1 "a".

ties higher than critical for the curved guide:  $v_{crit} = v_b(R/2d)^{1/2}$ , where  $v_b$  is the boundary velocity of the guide wall surface,  $R$  is the radius of curvature of the guide and  $d$  is the width of the guide.

Figure 3 demonstrates the influence of neutron capture and imperfectness of the surface on the transmission probability of straight vertical guides. All of the transmission curves have the characteristic minimum close to and above the guide boundary velocity. Such a behaviour results from different factors: at lower velocities the loss coefficient is low, at higher velocities the number of VCN reflections before arrival at the guide end decreases due to decreasing glancing angle of incidence.

Figure 4 shows the transmission through "realistic" curved guides of different curvatures. For comparison (curve 1) the



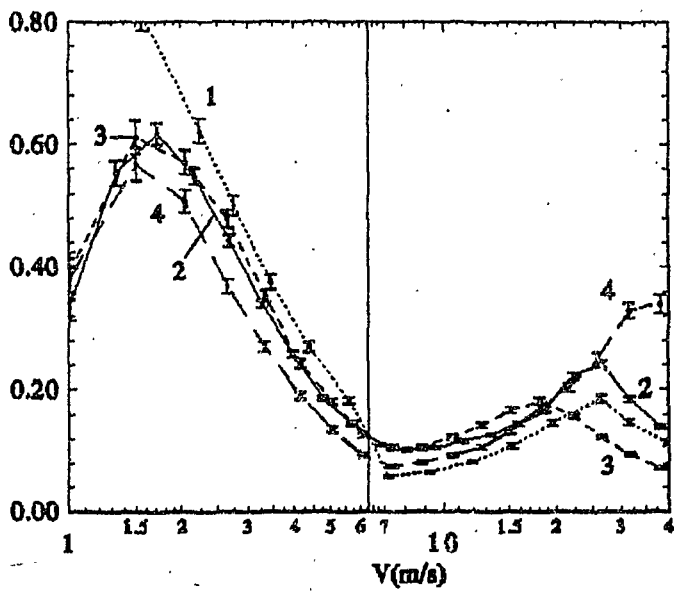


Fig.4 The arrival velocity dependence of neutron transmission through "realistic" curved guides in fig.1 (capture coefficient  $\eta = 5 \cdot 10^{-4}$ , surface roughness parameters  $\sigma = 30 \text{ \AA}$ ,  $T = 250 \text{ \AA}$ ): 1) horizontal guide with configuration "b", the transmission is normalized to the ideal straight horizontal guide; 2) vertical configuration "b"; 3) the same for configuration "c"; 4) the same for configuration "e". The normalization in curves 2-4 is as in fig.3.

transmission through a horizontal guide with the configuration "b" in fig.1 is shown. Higher UCN losses for configuration "e" guide (curve 4) are due to a larger length of this guide with a radius of curvature 7 m.

Figure 5 illustrates the effect of using supermirror neutron guides [12, 13, 14] on the VCN transmission probability. To simulate VCN transport in supermirror guide we used (approximate) experimental regular reflectivity parameters of Ni-Ti supermir-

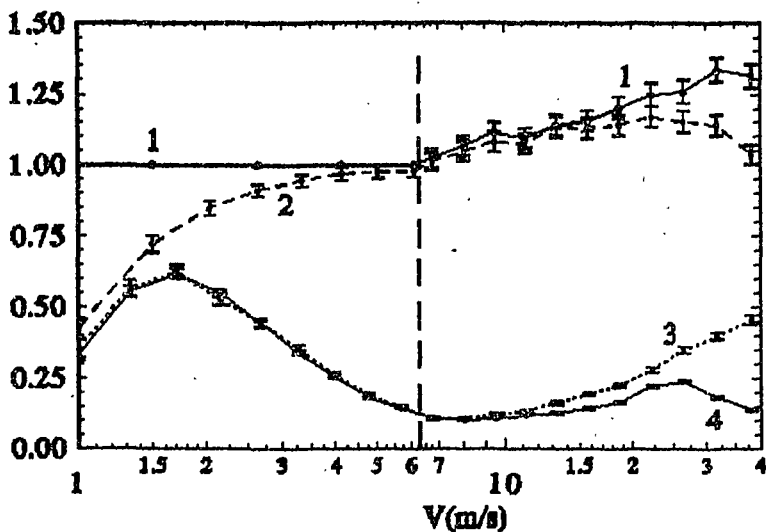


Fig.5 The arrival velocity dependence of neutron transmission through supermirror guides in fig.1: 1) configuration "a", ideal surface; 2) configuration "b", ideal surface; 3) configuration "b", capture coefficient  $\eta = 5 \cdot 10^{-4}$ , surface roughness parameters  $\sigma = 30 \text{ \AA}$ ,  $T = 250 \text{ \AA}$ ; 4) the same without the supermirror. The normalization as in fig.3 was made to transmission through ideal guide of configuration "a".

ror with 80 layers from fig.2 of the paper [14]. It was possible to foresee that for stored UCN, no gain in the transmission for neutron guide with an increased reflectivity of neutrons with energies above the boundary energy of the storage chamber could be expected (regardless vertical or horizontal guide is used). As can be seen from fig.5 the gain in the transmission is disappointingly low even for higher neutron velocities up to  $25 \text{ m/s}$ . Supermirror neutron guides are effective only for much higher velocities and a low number of reflections during neutron transport.

Figure 6 shows the (normalized to storage in an infinite volume through the ideal straight neutron guide) number of neu-

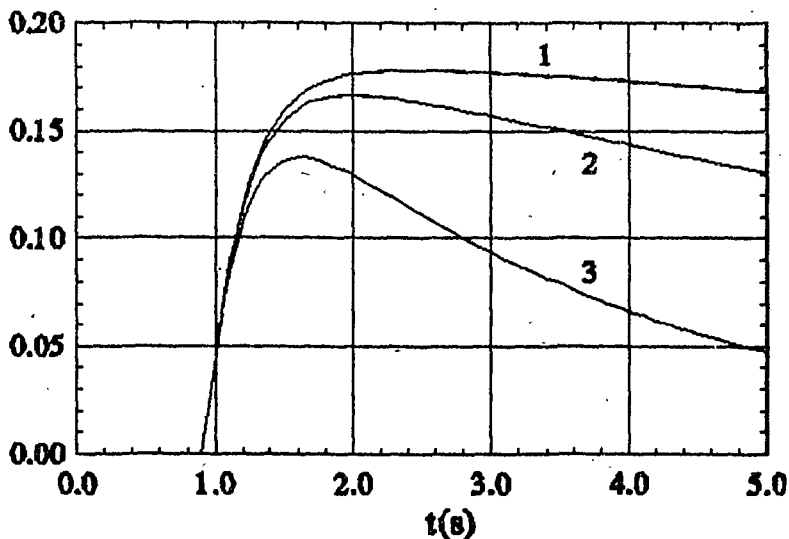


Fig.6 The time dependence of filling the storage volume with UCN through the guide of configuration "b",  $\eta = 5 \cdot 10^{-4}$ , surface roughness parameters  $\sigma = 30 \text{ \AA}$ ,  $T = 250 \text{ \AA}$ :

1) storage volume - 125l, 2) 40l, 3) 10l. The normalization was performed to one neutron in the maxwellian spectrum of the interval of the starting velocities of neutrons which can be stored in the infinite volume chamber through ideal guide of configuration "a".

trons stored in chambers with the volume  $V = 125l$ , 40l or 10l as a function of the time interval after the neutron source pulse.

If to close the shutter at the entrance to the storage volume, one can choose the spectrum of UCN stored in the chamber by varying the moment of shuttering. This can be performed because UCN with larger velocities arrive at the chamber earlier and, according to (12), also leave it earlier. This is illustrated in fig.7, where the spectral results of the Monte Carlo simulation of UCN storage are shown for different moments of closing the shutter.

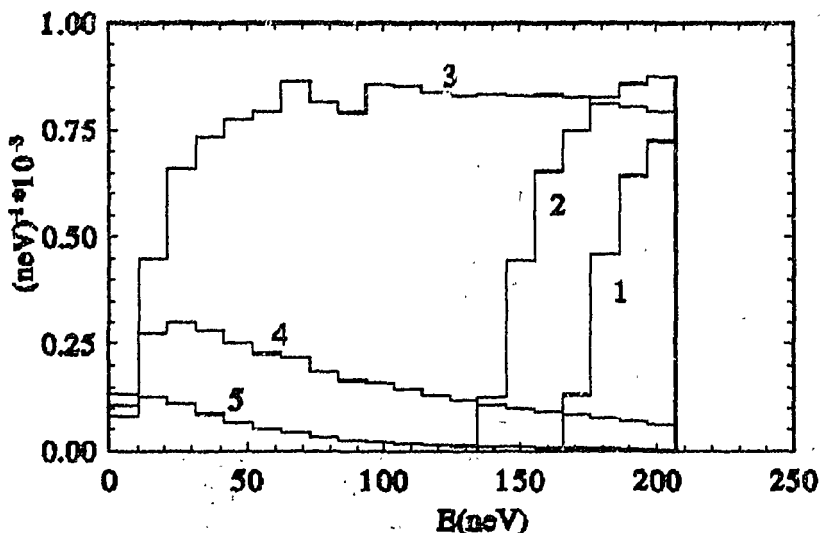


Fig.7 The stored UCN spectra for different shuttering moments  $t$  after the neutron pulse, guide configuration "b", surface roughness parameters  $\sigma = 30 \text{ \AA}$ ,  $T = 250 \text{ \AA}$ : 1)  $t = 0.95s$ , 2)  $t = 1.0s$ , 3)  $t = 2s$ , 4)  $t = 10s$ , 5)  $t = 20s$ .

The efficiency of such spectral filtering is higher in the vertical case than in horizontal case [1]. This is due to a more directed angular distribution of neutrons during their transport through a vertical neutron guide and, therefore, better time and space separation of neutrons with different velocities.

## 4 Conclusion

The results of the Monte Carlo simulation of VCN transport in curved vertical neutron guides show that for neutron guides with realistic surface roughness, the transmission through guides of practical length is quite acceptable. Calculations showed significant difference in the spectral dependence of transmission probability between vertical and horizontal cases and also better UCN

storage characteristics through vertical neutron guides as compared to the horizontal guides. The supermirror guides do not show better results for VCN transmission and UCN storage as compared to ordinary neutron guides. The reported results may be useful for possible realization of nonstationary UCN storage at the aperiodic pulse reactor.

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Моделирование методом Монте-Карло нестационарного транспорта очень холодных и ультрахолодных нейтронов в вертикальных нейтроноводах и накопления ультрахолодных нейтронов

Представлены результаты моделирования методом Монте-Карло транспорта очень холодных и ультрахолодных нейтронов в прямолинейных и криволинейных нейтроноводах прямоугольного сечения при наличии потерь нейтронов из-за захвата и диффузного рассеяния на неидеально гладкой отражающей поверхности стенок нейтроновода. Строго учитывалось гравитационное замедление нейтронов и искривление траекторий нейтронов. Проведено моделирование нестационарного накопления ультрахолодных нейтронов в экспериментальных камерах при использовании аperiodических импульсных нейтронных источников.

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Monte Carlo Simulation of the Nonstationary Transport of Very Cold and Ultracold Neutrons in Vertical Neutron Guides and the Storage of Ultracold Neutrons

The results are presented of a Monte Carlo simulation of the transport of very cold (VCN) and ultracold neutrons (UCN) in straight and curved vertical neutron guides with a rectangular cross section in the presence of neutron losses due to neutron capture and diffuse scattering on imperfectly smooth reflecting surface of the guides wall. The gravitational neutron deceleration and bending of neutron trajectories is taken into account rigorously. The nonstationary storage of UCN in experimental chambers is modelled for a low periodic or aperiodic pulse neutron source.

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

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