ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

95-106

E3-95-106

G.F.Gareeva, Al.Yu.Muzychka, Yu.N.Pokotilovski[1]

# MONTE-CARLO SIMULATION OF NONSTATIONARY TRANSPORT OF ULTRACOLD NEUTRONS IN HORIZONTAL NEUTRON GUIDES AND THE STORAGE OF ULTRACOLD NEUTRONS

Submitted to «Nuclear Instruments and Methods»

[1]E-mail: POKOT@nfsun1.jinr.dubna.su

1995

# 1 Introduction

Reflecting guide tubes [1, 2] for channelling of slow neutrons from a neutron source to experimental installations are now common facilities in many laboratories [3]. The transmittance of the neutron guides is determined by the reflecting properties of the guide surface: the probability of neutron loss (neutron capture and inelastic scattering) and of non-specular reflection per neutron encounter with the reflecting walls. Non-specular reflection, in the case of UCN transport in the neutron guides, causes (besides the mentioned losses) a time delay in the neutron arrival at the end cross section of the guide tube.

The effect of the imperfectness of the guide walls on the transmission of thermal and cold neutrons through the neutron guides has been considered in different publications [2], [4-13]. In most, the approach, especially for thermal neutrons, is rather simplified: the neutron loss probability per reflection is assumed to be independent of the neutron wave length and glancing angle to the reflecting plane below the critical angle. The exit intensity $I$ in this case contains the product of reflectivitities after each particular reflection: $I = I_0 \cdot \bar{R}^{\bar{n}}$, where $I_0$ is the neutron intensity at the entrance to the neutron guide, $\bar{R}$ is the mean reflection probability, and $\bar{n}$ is the mean number of reflections along the neutron path. The last figure is calculated from geometric considerations. For the calculation of $\bar{R}$ in [6, 7, 9] a more detailed and rigorous treatment of the effect of surface roughness on the angular distribution of imperfectly reflected cold neutrons was presented.

The spreading of UCN in neutron guides has some peculiarities. In the case of non-specular reflection, the neutron with a probability very near to unity survives in the neutron guide, but in some cases may return to the neutron source. The UCN transmission of neutron guides has been measured in several works [14-17], and theoretical analysis of the problem was performed in [14], [18-20]. Usually, the analysis was made in the frame of one dimensional diffusion theory in the one-velocity approximation or in supposition that the reflected intensity is a sum of the specular and diffuse components with corresponding weights. In [18-21] the Monte Carlo computations were performed for the transmission of UCN through neutron guides.

The nonstationary spreading of UCN in neutron guides was observed in two experiments. Robson [22] measured the time decay of UCN intensity at the end of a 5m neutron guide after a sharp shut down of the reactor. From the decay time ($\sim 2sec$) it was concluded that the probability of a diffuse reflection per encounter did not exceed 10%. In the experiment [16] the time dependence of UCN intensity was measured at the end of a stainless steel and glass neutron guides after the sharp opening of the shutter located between the detector and the UCN source. The qualitative interpretation of the experiment [16] was presented in [23] in the frame of the one velocity diffusion approximation and on this ground, the observed peak in the measured time distribution was explained. For a more realistic quantitative description of the nonstationary transport of UCN, this type of approximation is not valid.

Computer simulation of nonstationary transport may be interesting



from two points of view. First, analysis of the experimental arrival time distributions, when short bunches of UCN are injected at the entrance of the neutron guide, can help in extracting the parameters of the wall surface (probabilities of specular and diffuse reflection and neutron loss per collision, and possibly the characteristics of diffuse reflection) more unambigously than from mere stationary transmission measurements. Second, this analysis is useful for realizing the recently proposed method [24] of UCN storage using low repetition pulse neutron sources for their production.

## 2 Elastic scattering of UCN from rough surfaces

The reflection of slow neutrons by rough surfaces has been studied theoretically and experimentally in the last two decades. It was conceded that, in general, the reflected intensity consists of two parts: specular and diffuse, the last component having an angular distribution, depending on the surface properties. It is evident that the task of predicting an exact reflection law without having complete information about the roughness of the reflecting surface is impracticable. Therefore, usually some approximations are made regarding the general character of surface roughness, which describes the irregular deviations of the surface from the ideal plane by the autocorrelation function:

$$f(\vec{\delta}) = \langle \xi(\vec{\rho}) \cdot \xi(\vec{\rho}\,') \rangle = \lim_{S \to \infty} \frac{1}{S} \int_D \xi(\vec{\rho}) \cdot \xi(\vec{\rho} + \vec{\delta}) d^2\vec{\rho}, \quad (1)$$

or by the function connected with it:

$$g(\vec{\delta}) = \langle [\xi(\vec{\rho}) - \xi(\vec{\rho}\,')]^2 \rangle = 2 \cdot [\langle \xi^2(\vec{\rho}) \rangle - f(\vec{\delta})]. \quad (2)$$

This correlation function represents the statistical characteristics of the random function $\xi(\vec{\delta})$-deviation in the height of the surface at coordinate $\vec{\rho}$ from the mean value $\langle \xi(\vec{\rho}) \rangle = 0$.

The most natural form of $f(\vec{\delta})$ is:

$$f(\vec{\delta}) = \sigma^2 \cdot exp(-\delta^2/T^2), \quad (3)$$

where $\sigma = \langle\xi^2\rangle^{1/2}$ and $T$ are the mean square amplitude and the correlation length, respectively. The last value characterizes the mean square slope of roughness: $\alpha = 2 \cdot \sigma/T$.

Several authors have used this description of surface roughness for calculating (in the simple or distorted wave Born approximations) the probability of specular and diffuse reflections and of the diffusively scattered intensity as a function of the wave vector transfer $(q_z, q_\beta)$. These results (see [25, 26] and references therein) are applicable when: 1) $q_z \geq 2k_b$, where $k_b = (4\pi Nb)^{1/2}$ is the boundary wave vector of the surface material - the wave vector of the neutron for which the critical glancing angle of total reflection is equal to $\pi/2$, and 2) the difference from unity of the refractive index $n$ of the reflecting medium: $1 - n = bN/2\pi k^2$ is a very small quantity, e.g., when the total reflection from the surface is weak. Here $k$ is the wave vector of the neutron, $b$ is the scattering length of the atoms of the medium, and $N$ is atomic density of the medium. The formulas obtained in these works are appropriate for interpreting typical reflectometric experiments with thermal and cold neutrons, where the information about surface characteristics is obtained from analysis of specular reflectivity curves as a function of transferred momentum at large $q_z$ and low reflectivity. They are not appropriate for describing UCN reflection, when the probability of reflection is near unity. Steyerl [6] and Ignatovich [8] approached the problem of UCN reflection from a rough surface using the Green function method. They obtained coincident results for the case of micro-roughness: $k_z\sigma \leq 1$, which is interesting for the reflection of UCN from high quality mirror surfaces. Their result for the wave vector transfer dependence of diffuse reflection probability has the form:

$$w_{d.r.}(\Omega_0, \Omega) = \frac{1}{\pi} k^4 cos\theta_0 \cdot cos^2\theta \cdot \sigma^2 \cdot T^2 \cdot exp\left(-\frac{(\vec{k}_{\parallel} - \vec{k}_{0\parallel})^2 \cdot T^2}{4}\right), \quad (4)$$

where $k$ is the wave vector of the incident (and reflected) neutron, $\vec{k}_{\parallel 0}$ and $\vec{k}_{\parallel}$ are the parallel to the surface plane components of incident and scattered wave vectors, respectively, so that

$$(\vec{k}_{\parallel} - \vec{k}_{\parallel 0})^2 = k^2(sin^2\theta_0 + sin^2\theta - 2sin\theta \cdot sin\theta_0 \cdot cos(\phi - \phi_0)). \quad (5)$$



Here $\theta_0$ and $\theta$, $\phi_0$ and $\phi$ are the polar and azimuth angles of the incident to the surface normal and reflected neutrons, respectively. This expression has some important features: decreasing of the probability of diffuse reflection with $\theta_0 \rightarrow \pi/2$, a fulfilment of the requirement of the detailed balance principle, expressed in the term $cos^2\theta$ [18, 28], and concentration of the diffusively scattered intensity around the specular solid angle $(\theta, \phi)$. Integrating (4) over $\Omega$ gives the total probability of diffuse reflection:

$$\Delta = \int w_{d.r.}(\Omega_0, \Omega) d\Omega. \quad (6)$$

For

$$\lambda = 2\pi/k \cong 600 \text{ Å } (v \cong 5m/s), \quad \sigma \cong 25 \text{ Å},$$
$$T \cong 500 \text{ Å}, \quad \theta_0 \cong \pi/4, \quad \Delta \cong 0.1 \quad (7)$$

Expression (4) was used to describe the transmission of cold neutrons through a neutron guide in [7, 9] and of UCN in [19], and was experimentally verified [10] by the measurement of the angular distribution of cold neutrons emerging from straight neutron guides made of plexiglas and glass panes – both with $0.2\mu m$ evaporated Ni.

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

Expression (4) is applicable only for very smooth surfaces. No good simple theory exists for a description of diffuse scattering from a rough surface, when $k\sigma \geq 1$, which is convenient for Monte Carlo simulation of nonspecular reflection. It is known [27] that the probability of specular reflection from a rough surface is:

$$w(\theta_0) = exp(-2k^2 \cdot \sigma^2 \cdot cos^2\theta_0) \quad (8)$$

and is small except at very small glancing incident angles $(\theta_0 \simeq \pi/2)$. We used a simple model of diffuse reflection for this case – isotropic diffuse reflection – when the angular distribution has the form:

$$dw_{d.r.} = \Delta \cdot cos\theta \cdot d\Omega, \tag{9}$$

and also a more realistic kind of diffuse reflection:

$$dw_{d.r.} = \Delta \cdot cos\theta_0 \cdot cos^2\theta \cdot d\Omega. \tag{10}$$

The distribution (9) may approximately correspond to a macroscopically very rough surface, when the reflection angle does not depend on wave length nor incident angle of the neutron (except at small grazing angles, when the reflected intensity is not symmetrical with respect to the surface normal). The distribution (10) is the limiting case of (4) when $(\vec{k}_{||} - \vec{k}_{0||})^2 \cdot T^2/4 \ll 1$. In this case $\Delta = k^4 \cdot \sigma^2 \cdot T^2/\pi$.

Neither of these cases give the predominant diffusively reflected intensity around the specular angle (which takes place in our example (7), where the angular width of this angular distribution concentrated around the specular reflection is $\sim 0.4$). Therefore, we expect that the results of the simulation of nonstationary transport for this choice of the angular distribution of UCN after reflection will demonstrate larger time delays and neutron losses than in the case (4) at the same values of total diffuse scattering probability.

Two kinds of angular distribution of neutrons at the entrance apperture of the neutron guide were chosen: isotropic

$$dw_s \sim d\Omega, \tag{11}$$

which corresponds to a thin (transparent to UCN) voluminous neutron source with reflecting walls, and a more realistic cosine distribution

$$dw_s \sim cos\theta d\Omega, \tag{12}$$

which corresponds to a surface or thick voluminous UCN source.

With a neutron guide assumed to be horizontal and having a rectangular cross section $(6 \times 8cm)$, and a length $L = 6m$, the neutron spectrum usually has the form

$$\begin{aligned} f(v) &= 3v^2/(v_{2b}^3 - v_{1b}^3), \quad \text{if} \quad v_{1b} < v < v_{2b}, \\ f(v) &= 0, \quad \text{if} \quad v < v_{1b}, \quad \text{or} \quad v > v_{2b}. \end{aligned} \tag{13}$$



It corresponds to the beginning of the Maxwellian spectrum with a lower boundary $v_{1b}$ and an upper boundary $v_{2b}$; $v_{1b} = 320cm/s$ - for a possible aluminium window membrane of the UCN source, $v_{2b} = 600cm/s$ - coincides with the boundary velocity $v_b$ of the neutron guide (e.g., stainless steel). The spreading through neutron guides of neutrons with velocities greater than the boundary velocity of the guide's surface is not considered in this paper. Our main interest here is the simulation of transport of UCN that can be stored in material bottles.

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

$$\mu(v, \theta) = 2\eta \frac{v \cdot cos\theta}{v_b} \Big/ \sqrt{1 - \left(\frac{v \cdot cos\theta}{v_b}\right)^2}. \tag{14}$$

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

The order of simulation of the UCN trajectories was the following: at the beginning, the point of the UCN emergence (at the moment $t = 0$) into the neutron guide was drawn with equal probability on the entrance cross section of the neutron guide, velocity according to (13) and angle of emergence according to (11) or (12). At the next stage, the intersection plane was found and the angles of incidence, the intersection point coordinates, the length of the free flight and time of flight, after which the verification was performed of whether the neutron was captured according to (14). If the neutron survived then verification was made about the type of reflection: specular or diffuse. The corresponding angles of diffuse scattering were drawn according to (4), (9) or (10) and the cycle was repeated. The history of the neutron was set as finished if it was captured or its trajectory intersected the entrance or exit cross section of the neutron guide. The number of neutrons for each destiny variant and the total time of travel for every neutron reaching the exit apperture were summed.

For the simulation of the storage of UCN in experimental volumes at the end of the neutron guide (fig.1), it was supposed that the life time of the neutron in the storage chamber can be written as

$$\tau = 4V/sv, \tag{15}$$

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

# 4 Results of calculations

Three configurations of neutron guides were used for the computer simulation: straight, $\pi/2$ - bent and S - shaped (fig.2). The forms of the bent-neutron guides were chosen from practical demands: there are some advantages in bending neutron guides to a small radius of curvature – the possibility of using short guides and moderate radiation shielding.

Some results of calculations are shown in figs.3-5. All the calculations are based on not less than 1,000 histories for each case of calculation of the arrival time distribution (up to 10,000 histories in some cases). The curves show the integral arrival time distributions - quantity of neutrons, normalized to one neutron emerging into the neutron guide and arriving at the end of the neutron guide before the moment $t$.

For monochromatic and monodirectional incoming neutrons, the change in the arrival time distribution is caused by the transformation of the longitudinal component of the velocity into a transverse one (curves 1 and 2 in fig.3); in the S-shaped guide such mutual transformation takes place twice. For the cosine incoming angular distribution, this difference in the arrival time distribution is noticeable only at the beginning of the curve, but in general, the effect of the delay for the bent guides in comparison to the straight ones is smoothed out. Even the very sharp bending of the neutron guide when the internal (but not the external!) radius of curvature is $r_0 = 0$, the effect of bending is not very significant. At $r_0 \geq 30cm$ there is no difference in any of the arrival time distributions from the results for the straight neutron guide (for the cosine primary angular distribution).



Imperfectness of the neutron guide decreases the arrival rate as well as the overall quantity of the arrived neutrons (almost proportionally). The considered roughness parameters $\sigma = 30Å$, $T = 250Å$ or $500Å$ are quite realistic [6, 7] for polished metal surfaces. Rapid progress in the surface quality of neutron guides has been observed in recent years [3] and it is possible to have neutron guides with better characteristics. Curve 4 in figs.3 and 4 shows an example of a neutron guide with low quality: the case when 10% of the surface is macroscopically rough: the reflection law according to formula (9), $\Delta = 0.1$.

Values were also obtained for the probabilities of different neutron destinies during spreading along the neutron guides: the neutron loss in the wall - $w_l$, the probability of the neutron returning to the source – $w_b$, and the probability of the neutron arriving at the exit of the neutron guide - $w_a$.

Figure 1 shows the principle of method [24] proposed for storing UCN in experimental volumes using pulse neutron sources with well separated pulses (aperiodic pulse neutron sources, e.g., TRIGA type reactors). During the neutron pulse a high density of UCN is formed in the UCN converter (1). After spreading of the UCN bunch over the neutron guide (2) and partial storage in the experimental chamber (3), the shutter (4) located near the entrance window of the chamber is closed, UCN being locked in the chamber.

Fig.6 shows the normalized to one emitted neutron quantity of neutrons stored in the chamber for volumes $V = 20l$ and $50l$ and different lengths of the neutron guides: $6, 12$ and $18m$ as a function of the time interval after the neutron source pulse. It is seen that a significant part of the emergent UCN quantity may be stored using high quality neutron guides, especially when using sufficiently short ones. For guides with worse surface parameters, the quantities of stored UCN are proportionate to the corresponding arrival time data.

In this method, there is an interesting additional possibility to deliberately choose the spectrum of UCN stored in the chamber by varing the moment of closing the shutter. It can be performed due to the fact that UCN with greater velocity arrive at the chamber earlier, and according to (15) 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 of the shutter.

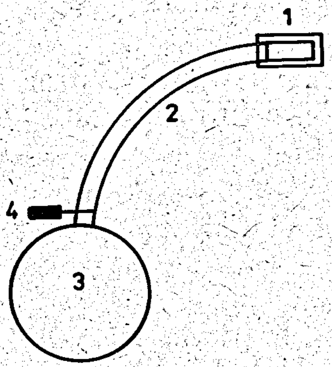


Fig.1 The principal scheme of storage of UCN at a pulse source:

1. UCN source
2. neutron guide
3. storage volume
4. UCN shutter

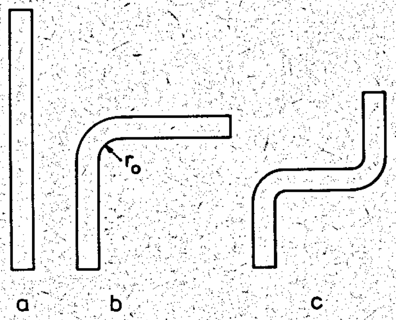


Fig.2 Configurations of the neutron guides used in the Monte Carlo simulations: a–straight, b–$\pi/2$-bent, c–S-shaped.



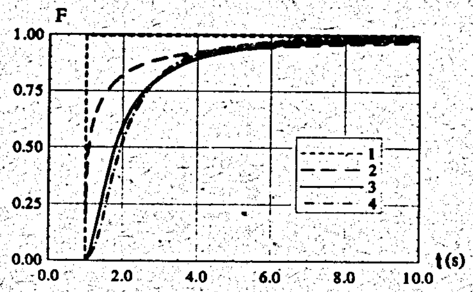


Fig.3 Integral arrival time distributions for an ideal neutron guide with a length of $6m$ without losses:

1. monochromatic neutrons with velocity $6m/s$ along the tube axis, straight neutron guide,
2. the same for 90°-bent neutron guide, $r_0 = 0$,
3. Maxwellian spectrum, eq.(13), with angular distribution at the entrance, eq.(12), straight neutron guide,
4. the same for S-shaped neutron guide, $r_0 = 0$.

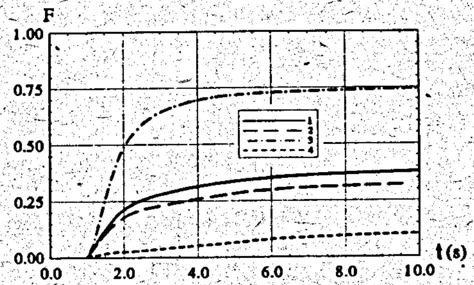


Fig.4 Integral arrival time distributions for the straight neutron guide with a length of $6m$, neutron spectrum eq.(13) and entrance angular distribution eq.(12):

1. $\eta = 5 \cdot 10^{-4}$, $\sigma = 30$Å, $T = 250$Å; $w_l = 0.11$, $w_b = 0.52$, $w_a = 0.37$.
2. the same, but $T = 500$Å; $w_l = 0.11$, $w_b = 0.56$, $w_a = 0.33$.
3. the same, but $T = 50$Å, coincides with simulation according to eq.(10) with $\Delta = 0.0124$; $w_l = 0.10$, $w_b = 0.16$, $w_a = 0.74$.
4. diffuse reflection according to eq.(9) with $\Delta = 0.1$; $w_l = 0.16$, $w_b = 0.73$, $w_a = 0.11$.

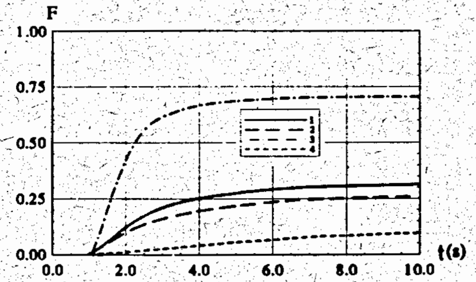


Fig.5 The same as in fig.4 but for the S-shaped neutron guide with a length of $6m$, $r_0 = 2cm$.

1. $w_l = 0.10$, $w_b = 0.57$, $w_a = 0.33$.

2. $w_l = 0.12$, $w_b = 0.60$, $w_a = 0.28$.

3. $w_l = 0.16$, $w_b = 0.11$, $w_a = 0.73$.

4. $w_l = 0.15$, $w_b = 0.75$, $w_a = 0.10$.

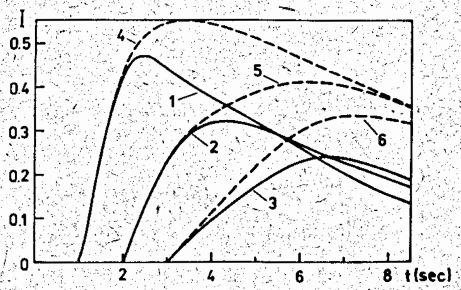


Fig.6 The time dependence of filling the storage volume with UCN through straight neutron guides with diffuse reflection according to eq.(10) with $\Delta = 0.0124, \eta = 5 \cdot 10^{-4}$: 1, 2, 3 – storage volume $20l$, lengths of the neutron guides are 6, 12 and $18m$ respectively; 4, 5 and 6 – storage volume $50l$, lengths of neutron guides are 6, 12 and $18m$, respectively.



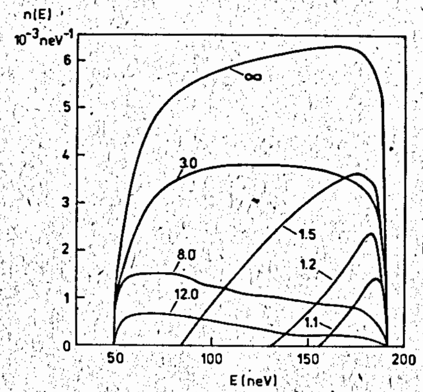


Fig.7 The stored UCN spectra after closing the shutter at different moments (*sec*) after the neutron pulse: guide length is $6m$, storage volume $20l$, diffuse reflection according to eq. (10) with $\Delta = 0.0124, \eta = 5 \cdot 10^{-4}$.

# 5 Conclusion

The results of the Monte Carlo simulation of the nonstationary transport of UCN show that for neutron guides with realistic surface roughness, the transmission through guides of practical length is quite acceptable and there is almost no dependence on the radius of bending curvature of the guides even at very small values of the radius. The calculations also show that the storage of UCN using aperiodic pulse neutron sources may be performed effectively with realistic guides.

# 6 Acknowledgments

One of authors (Yu.P) wishes to express his thanks to Dr. V.K. Ignatovich for discussions of the problem of UCN scattering from a rough surface.

## References


[1] J.Christ and T.Springer, Nucleonik, 4 (1962) 23

[2] H.Maier-Leibnitz and T.Springer, Nucl.Energy A/B 17 (1963) 217

[3] "Proc. Symp. on Thin-Film Neutron Optical Devices: Mirrors, Supermirrors, Multilayer Monochromators, Polarizers and Beam Guides, San Diego, USA, SPIE Proc. 988(1989), C.F.Majkrzak (ed.).

[4] B.Alefeld, J.Christ, D.Kukla, R.Scherm and W.Schmatz, Neutronenleiter, Jül-294-NP, (1965)

[5] B.Farnoux, B.Hennion, I.Fagot, Proc. 4th IAEA Symp. on Neutron Scatt. (Copenhagen 1968),353

[6] A.Steyerl, Z.Phys. 254 (1972) 169

[7] A.Steyerl, Nucl.Instr.Meth., 101 (1972) 295

[8] V.K.Ignatovich, JINR Commun. P4-7055 (1973)

[9] A.Steyerl, Nucl.Instr.Meth., 125 (1975) 461

[10] K.-J.Kugler, W.Paul and U.Trinks, Z.Phys. B39 (1980) 361

[11] D.F.R.Mildner, Nucl.Instr.Meth., A292 (1990) 693

[12] A.Schirmer and D.R.F.Mildner, Measur.Sci.Technol. 2 (1991) 1059

[13] D.Dubbers, Nucl.Instr.Meth., A349 (1994) 302

[14] V.I.Lushchikov, Yu.N.Pokotilovsky, A.V.Strelkov and F.L.Shapiro, Pis'ma ZhETF, 9 (1969) 40

[15] L.V.Groshev, V.N.Dvoretsky, A.M.Demidov, Yu.N.Panin, V.I.Lushchikov, Yu.N.Pokotilovsky, A.V.Strelkov and F.L.Shapiro, Phys.Lett., 34B (1971) 293

[16] A.I.Egorov, V.M.Lobashev, V.N.Nazarenko, G.D.Porsev and A.P.Serebrov, Yad.Fiz., 19 (1974) 300





[17] Yu.Yu.Kosvintsev, E.N.Kulagin, Yu.A.Kushnir, V.I.Morozov, and A.V.Strelkov, Nucl.Instr.Meth., 143 (1977) 133

[18] I.Berceanu and V.K.Ignatovich, Vacuum, 23 (1973) 441

[19] M.Brown, R.Golub and J.M.Pendelbury, Vacuum, 25 (1975) 61

[20] D.Winfield and J.M.Robson, Can.J.Phys., 53 (1975) 667

[21] W.Maysenholder, Nucl.Instr.Meth., 13 (1976) 291

[22] J.M.Robson, Can.J.Phys., 54 (1976) 1277

[23] V.K.Ignatovich and G.I.Terekhov, Nucl.Instr.Meth., 148 (1978) 585

[24] Yu.N.Pokotilovski, JINR Preprint E3-94-227, Nucl.Instr.Meth. A (1995) in press.

[25] S.K.Sinha, E.B.Sirota, S.Garoff and H.B.Stanley, Phys.Rev., B38 (1988) 2297

[26] R.Pynn, Phys.Rev., B45 (1992) 602

[27] F.G.Bass and I.M.Fuks, "Scattering of waves on a statistically non-flat surface", Nauka, Moscow, 1972, ch.VII (in Russian).

[28] V.K.Ignatovich, Izvestija Vuzov (Radiofyzika), 18 (1975) 1551 (in Russian).


**Received by Publishing Department on March 15, 1995.**