A numerical model of a coated capillary-plate thermal neutron collimator^{*}

TIAN Yang(田阳)^{1,2;1)} YANG Yi-Gang(杨祎罡)^{1,2} LI Yu-Lan(李玉兰)^{1,2} LI Yuan-Jing(李元景)^{1,2}

¹ Department of Engineering Physics, Tsinghua University, Beijing 100084, China ² Key Laboratory of Particle & Radiation Imaging (Tsinghua University), Ministry of Education, Beijing 100084, China

Abstract: A novel thermal neutron collimator was successfully fabricated by coating the inner surface of the capillary plate (CP) with gadolinium oxide using atomic layer deposition (ALD) technology. This CP-based collimator is efficient and compact. A numerical model is presented in the paper to estimate the main performance characteristics of the collimator and to optimize the design for specific applications. According to the results of the calculation based on currently available CPs, the FWHM of the collimator's rocking curve can be smaller than 0.15° while suppressing more than 99.9% of the incident thermal neutrons on the double wings of the curve. Such a coated CP is as thin as 1.25 mm or even thinner, providing high angular resolution with good transmission in a very limited space.

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1 Introduction

In the past few decades, neutron collimators of Soller slit type have been widely used in neutron scattering experiments [1, 2]. The basic idea of these collimators is to combine neutron absorbing materials with an array of slits or channels made from materials with high neutron transparency. There are several common requirements to achieve a high performance collimator, such as large length to width ratio, excellent geometric accuracy and high neutron transparency of the bulk volume. One of the current trends is to introduce a compact structure with a high degree of geometric accuracy, e.g. the one made with silicon wafer [2]. Based on this idea, Nova Scientific Inc. has manufactured the most compact one using a ¹⁰B or ^{nat}Gd doped micro-channel plate (MCP). In spite of the high collimating ratio obtained, the transparency is limited to around 63% due to the intrinsic porosity of the MCP [3].

To overcome this drawback while preserving the advantages of MCP, we developed a new compact neutron collimator based on a gadolinium-coated capillary plate (Fig. 1). A capillary plate is a by-product of MCP without inner surface treatment and electrodes intended for signal amplification, and is thus available at a much lower price. Traditionally, it is produced by drawing and fusing glass material to form a hexangular array of circular pores whose porosity is about 63%. The diameter D of the microchannel can be as small as 2 μ m. Although there are some limits during manufacturing, an L/D ratio as large as 250:1 is achievable. After coating the inner surface of the channels with ^{nat}Gd₂O₃, one can get a very compact collimator. The thickness of the plate (equal to channel length L) is about 1 mm or even smaller. Neutrons with a relatively larger incident angle θ are more likely to be absorbed in the coating layer, while the bulk material of the CP is almost transparent to neutrons, thus breaking the transparency limit of 63% set by the porosity of the CP/MCP.

In our first attempt, several hundred nanometers of $^{nat}Gd_2O_3$ were successfully coated on the inner

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¹⁾ E-mail: cycjty@126.com

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Fig. 1. The coated CP collimator. For a neutron beam with a certain direction (θ, φ) and uniform distribution within the rectangular cross section, there is a certain distribution of transmission probability within the cross section.

surface of the capillary plate using atomic layer deposition technology [4]. In the present paper, a numerical model of the new collimator is built and used to estimate the performance of the collimator and to help optimize the design.

2 Numerical model of the collimator

A model of the collimator is shown schematically in Fig. 1. The incident angle θ and azimuth angle φ are introduced to determine the direction of each neutron with respect to the coated CP system. For each fixed θ and φ , we use a uniform neutron beam with rectangular cross section to obtain the absorption distribution within the beam cross section.

The probability $P_{\rm e}$ for each incident neutron to escape from the coated CP (transmission probability) can be calculated as:

$$P_{\rm e} = \exp(-n_{\rm Gd}\sigma_{\rm Gd}T). \tag{1}$$

Here, $n_{\rm Gd}$ is the number of Gd atoms per unit volume within the ^{nat}Gd₂O₃ layer, $\sigma_{\rm Gd}$ is the neutron absorption cross section of ^{nat}Gd, and *T* is the total length of the neutron trajectory within the coating layer. In Eq. (1), only absorption by Gd is taken into account since the great absorption cross section of ^{nat}Gd (49700 b for 25.3 meV neutrons) makes the exponential absorption in the coating layer become dominant and suppresses the other interactions with the coated CP to a negligible level.

To determine the value of T, one can first calculate the length of its projection $T_{\rm p}$ on the head face of the CP (Fig. 2). T is equal to $T_{\rm p}$ divided by $\sin\theta$. In Fig. 2, the coordinates system lies on the head face of the CP towards the neutron beam. Each incident neutron can be characterized by four qualities: θ , φ , $x_{\rm s}$ and $y_{\rm s}$, where $(x_{\rm s}, y_{\rm s})$ is the intersection of the neutron trajectory with the coordinate plane. θ and φ are the incident angle and azimuth angle defined in Fig. 1. $(x_{\rm e}, y_{\rm e})$ is the intersection with another head face. The equation of the neutron trajectory's projection is as follows:

$$Ax + By + C = 0, \quad A = \sin\varphi,$$

$$B = -\cos\varphi, \quad C = y_s \cos\varphi - x_s \sin\varphi.$$
(2)



Fig. 2. The projection of the neutron trajectory on the head face of the CP.

The capillary plate can be treated as a rectangular array of many basic units, and is shown by the dotted lines in Fig. 2. The calculation processes of $T_{\rm p}$ are as follows: first, the units that have at least one intersection with the neutron trajectory are determined by $(x_{\rm s}, y_{\rm s}), (x_{\rm e}, y_{\rm e})$ and the equation Ax+By+C=0; second, the centers of all the ^{nat}Gd₂O₃ rings (numbered as 1, 2, \cdots , *i*, \cdots) involved in these units (five rings for each unit) are recorded and the reduplicates are discarded; third, the distance d_i between each center (x_{ci}, y_{ci}) of these rings and the line defined by Ax+By+C=0 using Eq. (3) is calculated; fourth, the

Vol. 36

half chord length L_i and l_i for the outer and inner circles of each ring *i* mentioned above using Eq. (4) is calculated; and finally, the values of $T_{\rm p}$ and T are given by Eq. (5).

$$d_i = \frac{|Ax_{ci} + By_{ci} + C|}{\sqrt{A^2 + B^2}}.$$
(3)

$$L_i = \sqrt{R^2 - d_i^2}, l_i = \sqrt{r^2 - d_i^2}.$$
 (4)

$$T_{\rm p} = 2\sum_{i} (L_i - l_i), \ T = T_{\rm p} / \sin \theta.$$
 (5)

The absorption of the coated CP for neutrons of a certain direction should be an average over different intersections with the CP. To calculate this average value, one can place the intersections uniformly within one unit in Fig. 2, i.e. to dwindle the beam in Fig. 1 to cover only one unit. The x and y intervals of the intersections can be chosen according to the thickness of the coating layer. In the following calculations in Section 3, the interval is determined as 1/20 of the thickness. $P_{\rm e}$ is the average value over one unit.

Our first experiment using the thermal neutron beam of the 49-2 swimming pool LWR of CIAE has verified the validity of the numerical model [4]. Monte Carlo simulation by Geant 4.9.4 was also carried out to estimate the effect of the other interactions with the CP. The model used is the same as that in Fig. 1. Fig 3 shows the calculation results for 25.3 meV neutrons by both the numerical model and the Monte Carlo simulation. The results agree well with each other. The average values of $P_{\rm e}$ within the 70 µm×70 µm cross section are 0.129 and 0.127, respectively.



Fig. 3. The distribution of $P_{\rm e}$ within the neutron beam cross section derived from the numerical model (a) and Geant4 (b). The channel diameter and L/D of the CP are 10 µm and 1:50, respectively. The neutron beam is the one shown in Fig. 1 with a cross section of 70 µm×70 µm. θ and φ are 1.5° and 15°. Here, $P_{\rm e}$ is not the average value. (c) shows the value of $P_{\rm e}$ along the diagonal of the cross section (d is the distance from the top left corner).

3 Calculation results and discussion

The performances of coated CPs with different dimensions were estimated by the above model. Capillary plates with a channel diameter of 5 µm and 10 µm are now commercially available in China. 2 µm MCP has also been reported by some foreign teams [5]. CPs with channel diameters of 2, 5 and 10 µm are covered in the calculation. As a current technical obstacle, an L/D of 250:1 is set as an upper limit. Although in our first attempt only the CP with a channel diameter of 10 µm and L/D of 50:1 was coated, it is easy to coat delicate structures with dimensions as small as 0.5 µm or even some tens of nanometers, and L/D as large as 1000:1. The following calculations all correspond to 25.3 meV thermal neutrons if the energy is not declared.

3.1 Transmission characteristics of the collimator

Compared with the Soller slit type, the coated CP collimator can collimate neutrons with all the different azimuth angles, and this is illustrated in Fig. 4. The symmetry of the CP's structure makes it enough to cover only 30 degrees of the azimuth angle. It is clear that the behavior of the collimator does not vary too much among different azimuth angles.

3.2 The model-predicted rocking curve

Traditionally, a rocking curve is used to evaluate the collimation efficiency, which is the neutron transmission probability $P_{\rm e}$ as a function of the rocking angle. As most neutron collimators only work in one axis, the rocking angle ω ($\omega > 0$) corresponds to ($\theta = \omega, \varphi_0$) in the coated CP system shown in Fig. 1, while the minus value $-\omega$ corresponds to ($\theta = \omega, -\varphi_0$). Here, φ_0 is a fixed azimuth angle determined by the axis where the collimator works. Because the performance depends very weakly on φ as stated above, we fixed the value of φ_0 at 30° in the rocking curve calculation for the sake of simplicity.



Fig. 4. The transmission characteristics of the collimator ($P_{\rm e}$ as a function of θ and φ). The channel diameter and L/D of the CP are 10 µm and 1:100, respectively. The coating thickness is 100 nm.

Figures 5 and 6 present some of the rocking curve results obtained using different parameters. There are two important qualities of the rocking curve. The first one is the FWHM, and the other is the rejection ratio $R_{\rm j}$, which is defined as the average value of $1-P_{\rm e}$ on the wings of the rocking curve. These two factors clearly reflect the collimating efficiency. The FWHM is mainly determined by the L/D ratio. Large L/Dresults in a sharp peak, i.e. small FWHM (see Fig. 5). Different thicknesses of the ^{nat}Gd₂O₃ layer give different rejection ratios. A CP with a thick coating layer can reject more neutrons on the wings of the rocking curve (see Fig. 6).

The rocking curve of doped MCP with 3 mole %^{nat}Gd₂O₃ is also included in Fig. 6. To get the result, $T_{\rm p}$ should be calculated by Eq. (6). The 3 mole % is the current upper limit of the doping ratio, and the main performance of the coated CP collimator is even better than that of the doped one (see the 200 nm CP). Moreover, the maximum value of $P_{\rm e}$ for the former is more than 90%, resulting in much larger transmission efficiency. This major advantage makes it advisable to stack two or three coated CPs to enhance the collimating effect at the expense of transmission efficiency.

$$T_{\rm p} = \sqrt{(x_{\rm s} - x_{\rm e})^2 + (y_{\rm s} - y_{\rm e})^2} - 2\sum_i L_i.$$
 (6)



Fig. 5. The predicted rocking curves for CPs with different L/D ratios. The 10 μ m channels are coated with 100 nm ^{nat}Gd₂O₃.



Fig. 6. The predicted rocking curves for CPs with different coating thicknesses and doped MCP. The channel diameter and L/D are 10 μ m and 1:250 for the coated CP and doped MCP.

3.3 Some useful results for the collimator design

In the design of a collimator based on the CP with a certain channel diameter, one should carefully choose the L/D ratio and coating thickness according to the requirements of the application. Table 1 lists the FWHM values for CPs with different channel diameters D and different L/D ratios, together with the coating thicknesses required by different rejection ratios. T_{99} and $T_{99.9}$ are the thicknesses required by rejection ratios of 99% and 99.9%, respectively.

Vol. 36

$D/\mu m$	L/D	$FWHM/(^{\circ})$	T_{99}/nm	$T_{99.9}/{\rm nm}$	$R_{\rm j0.1eV}(\%)$	
10	1:250	0.146	125	209	91.0	
	1:100	0.376	323	552	—	
5	1:250	0.141	120	202	92.2	
	1:100	0.362	314	535	—	
2	1:250	0.138	117	196	92.7	

Table 1. Some useful results for the collimator design.

Although the absorption cross section of gadolinium drops with the increase in neutron energy, it is still two orders greater (9003 b) than the scattering cross section (73.5 b) at 0.1 eV. Within this energy range (<0.1 eV), the numerical model is considered to be valid. Nevertheless, the rejection ratio will degrade. Table 1 also includes the calculated R_j for 0.1 eV neutrons ($R_{j0.1eV}$). The coating thickness is 200 nm. To achieve a 99% rejection ratio to 0.1 eV neutrons, a coating thickness of 600 nm is needed for the CP with an L/D ratio of 1:250.

The performance of the coated CP collimator can be further enhanced with the development of a CP manufacturing technique. The new silicon CP technology has made it possible to produce a CP with an L/D as large as 1:300 [6]. A CP with ultra-small channels has also been highlighted. However, capillary plates with a small channel diameter (5 µm or 2 µm) are much more expensive. They also bring some drawbacks to the ALD coating, e.g. a possi-

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ble increase in the time required for each cycle [7]. Although the collimating effect is almost the same (Table 1), CPs with ultra-small channels are more desirable in high resolution neutron imaging applications because at the level of some tens of micrometers, the effect of the distribution of $P_{\rm e}$, as illustrated in Fig. 3, is outstanding for 10 µm CPs.

4 Conclusion

According to the results from the numerical model, the most common 10 μ m channel diameter CP, with an L/D of 1:250, has a rocking curve with an FWHM as small as 0.146° and suppresses 99.9 % of the thermal neutrons on the double wings after being coated on the inner surface with about 200 nm of ^{nat}Gd₂O₃. Such a coated CP is as thin as 1.25 mm, providing high angular resolution with good transmission in a very limited space.

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