Optimization of a polarizer device for SANS-2 instrument at the PIK reactor

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Abstract. A polarizer of V-cavity type for small angle diffractometer was considered. The device performance was simulated using McStas ray tracing package with the input parameters for supermirrors of PNPI home production (CoFe/TiZr, $m = 2.13$). Two replaceable devices with lengths 0.75 m and 1.8 m are proposed to cover the wavelength range 4–25 Å with beam polarization not less than 95%.

Introduction
A small-angle neutron scattering diffractometer SANS-2 was transferred to Petersburg Nuclear Physics Institute (PNPI) from Helmholtz Zentrum Geesthacht (HZG), Germany, after the FRG reactor was shutted down. At the moment the instrument is being reconstructed for installation at the PIK reactor, Gatchina, Russia. Among other parts, a new polarizer for SANS-2 has to be developed. When operated at FGR reactor SANS-2 used the reflection-type bender as a polarizer. That device provided inconvenience in use since the switching to polarized neutrons mode caused movement and alignment of the whole 40 m long instrument. Furthermore, the transmission rate was also an issue: the bender provided transmission not more than 70% due to losses in glass walls. Thus the construction of a new transmission polarizer is required. The polarizer of V-cavity type \cite{1, 2, 3} was chosen for simulations since a single mirror appeared to be too long for assembly and adjusting considering a spectral range specified, and bender type devices couldn’t increase the transmission compare to the old device.

The reason why we consider the device based on polarizing supermirrors is the following. Compare to the $^3$He polarizers \cite{4} the supermirrir polarizer is relatively simple in construction and needs no service when being used. The technology of polarizing supermirrors production is available at the moment at PNPI. The $m$-values available at the moment are not extremely high, but these coatings were never applied for the wide spectral range optics before, and the aim of this work is to set whether is it possible to implement.

1. Input parameters
The neutron ray-tracing package McStas \cite{5, 6} was used to calculate the flux and polarization after the polarizer. A sketch of a model used is shown in the figure 1. As the input parameters we used a real spectrum of HEC-3 reactor beam tube equipped with cold neutron source (as a source see Fig. 1) and a model of neutron guide being now developed for SANS-2 ($m = 1$,
cross-section $30 \times 30 \text{ mm}^2$). To simulate the instrument optical scheme we used a velocity selector component and a collimation line consisted of 8 exchangeable sections of 2 m length corresponding to SANS-2 layout.

![Source Neutron Guide Velocity Selector Polarizer Collimation line (8 exchangeable guide/non-optics sections) Sample position](image)

**Figure 1.** A sketch of model used in simulations.

Corresponding to McStas reflectivity description [6], a number of parameters is to be set: critical Q-vector $Q_c$, supermirror index $m$, supermirror regime reflectivity slope $\alpha$ and $mQ_c$ drop width $W$. These values were obtained from the best fit of the experimental curves for CoFe/TiZr multilayer structures, produced by PNPI [7, 8]. These parameters are given in the table 1. In this table $R^\pm$ stands for two components of polarization, and $R^{\pm}_{\text{dbl}}$ is the reflectivity of the double coated (on both sides) supermirror we used in simulations. To take into account the reflections from both sides, we added the contribution to the intensity the fraction which was once transmitted and then reflected. Mathematically this simple assumption holds

$$R^{\pm}_{\text{dbl}} = R^{\pm} + (1 - R^{\pm})R^{\pm},$$

and as a result it sufficiently changes the slope $\alpha$ (see third raw in table 1). Different slope gives new improved magnitude of the cut-off reflectivity $R_m = 0.90$ instead of $R_m = 0.75$ for single coated supermirror. For the negative component $R^-$ there are no changes since a reflectivity curve has no sloping region corresponding to multilayer structures: the reflectivity is 0.99 up to $Q_c$ and then drops dramatically.

| Pol. comp. | $Q_c [\text{Å}^{-1}]$ | $m$ | $R_0$ | $\alpha [\text{Å}]$ | $W [\text{Å}^{-1}]$ |
|------------|-----------------|-----|-------|-----------------|-----------------|
| $R^+$      | 0.0219          | 2.13| 0.995 | 13.87           | 0.00187         |
| $R^-$      | 0.0102          | 1   | 0.99  | 0               | 0.001           |
| $R^{\pm}_{\text{dbl}}$ | 0.0219 | 2.13| 0.995 | 3.43            | 0.00187         |

The polarizer should provide polarization no less than 95% with the maximal transmission in the whole spectral range which is used by the instrument. SANS-2 is planned to operate in the wavelength range from 4.5 to about 20 − 25 Å. Covering such a wide range with one optical polarizer with in-house coating $m = 2.13$ was found impossible as it is shown below, so we came to two exchangeable polarizers for short and long wavelength ranges. For optimization of the monochromatic beam we used a velocity selector model adjusted to 4.5 Å and to 10 Å with 10% resolution.
2. Results and discussions
First we optimized the short wavelength range polarizer. Figure 2 shows the dependence of polarization versus the polarizer length for five different beam collimations. The minimum polarizer length corresponds to the value of $L = 1.8$ m where all the curves saturate. This length is directly coupled to the inclination angle of supermirror plate. The corresponding angle is 8.3 mrad. Figure 3 shows the spectral dependence of polarization. It is well seen that such polarizer provides good polarization in the wavelength range from about 4.5 Å to about 11 Å for all the values of the beam divergence.

Figure 2. Polarizer length dependence of polarization for different beam collimations for $\lambda = 4.5$ Å.

Figure 3. The polarization spectral dependence of 1.8 m long polarizer.

Figures 4 and 5 show transmission spectral dependencies for $R^-$ and $R^+$ components respectively. As it is clearly seen from these figures, this polarizer performs well in the range from about 4.5 to about 10 Å. A limit at shorter wavelengths is induced by the $R^+$ reflectivity drop-off at high $Q$-values: the short wavelength neutrons are not reflected at all and the polarization degree in the transmitted beam is low. In the opposite way, the long-wavelength bound is caused by the full-reflectivity area in silicon: both spin components are reflected and the transmission of the device drops to zero. It is not the case for the non-collimated beam ($\gamma = \pi$ rad), since in divergent beam there still are trajectories with falling angle exceeding critical angle. Therefore

Figure 4. Spectral dependence of the transmission of $R^-$ component of polarization.

Figure 5. Spectral dependence of the transmission of $R^+$ component of polarization.
it is very important to optimize optics considering individual instrument beam requirements and setting divergence bounds is essential.

Exactly the same procedure was done for the second polarizer optimized for the long wavelength range (from about 10 to about 20 Å). Corresponding pictures are figures 6-9.

![Figure 6.](image1.png)  
Figure 6. Polarizer length dependence of polarization for different beam collimations for $\lambda = 10$ Å.

![Figure 7.](image2.png)  
Figure 7. The polarization spectral dependence of 0.75 m long polarizer.

![Figure 8.](image3.png)  
Figure 8. Spectral dependence of the transmission of $R^-$ component of polarization.

![Figure 9.](image4.png)  
Figure 9. Spectral dependence of the transmission of $R^+$ component of polarization.

The optimal length of the second polarizer found to be 0.75 m. This corresponds to the supermirror inclination angle of 20 mrad.

3. Conclusions
Using the coatings considered (production available at PNPI at the moment) doesn’t allow to make a single polarizer for a wide spectral range. Our calculations show that to cover the wavelength range from about 4.5 to about 25 Å two exchangeable devices are needed. The first one (figures 3, 4, 5) operates in a range from about 4.5 to about 10 Å, the second one (figures 7, 8, 9) fits the range from about 10 up to about 25 Å. Both polarizers provide good beam polarization — not less than 0.95 for any neutron wavelength in the range $4.5 \div 25$ Å. The transmission of negative spin component is also satisfactorily high: not less than 0.95 for
the major part of the operating range and not less than 0.7 at the range edges. It is worth to note that the operation of PNPI in-house supermirror coatings was first simulated and shown to be applicable in optics for wide spectral range.

In principle it is possible to cover entire range of wavelengths with the only one polarizer, but for this purpose one need the supermirror with higher $m$ coefficient. We chose as example a supermirror with $m = 5.5$ commercially available at the moment and we performed simulations using parameters provided by SwissNeutronics [9].

![Figure 10](image-url)  
**Figure 10.** Polarization spectral dependence for V-cavity type polarizer with $m = 5.5$.

![Figure 11](image-url)  
**Figure 11.** Transmission spectral dependence for V-cavity type polarizer with $m = 5.5$.

Figures 10-11 show the performance of V-shaped polarizer of 0.9 m length. As one can see from these pictures, such a device could perform well in the entire desired wavelength range (from 4.5 to about 20 Å).

One thing should be pointed out. The polarization degree for polarizer with high-$m$ supermirror is few percent less compare to the one based on the lower $m$ coating. This is caused by the lower reflectivity in supermirror region (from $Q_c$ to $mQ_c$) for $R^+$ component. Higher $m$ obviously makes this region wider, but the reflectivity here is lower. The transmission for negative spin component ($T_-$) supposed to be around 1, and it remains the same for both types of supermirrors (see fig. 4 for $m = 2.13$ and fig. 11 black squares and red circles for $m = 5.5$). For positive spin component ($T_+$) transmission should be as low as possible, but for supermirror with $m = 5.5$ it increases compare to the one with $m = 2.13$ (see fig. 5, and fig. 11 blue and green triangles). The higher $T_+$ component becomes, the lower polarization it gives. In our case it is not the most important factor since we initially established the restriction for polarization at 0.95, but in some applications of supermirror polarizers it could be significant.

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