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Design of W/Si supermirror by block method

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ABSTRACT

In X ray region, the supermirror can provide better optical performance than metal substrate or two-layer mirror. W/Si supermirrors are designed in 0.2–10 keV by block method. These mirrors have big grazing incidence angles of 1.0, 1.4, and 1.7 degrees, which is the most important characteristic in our job. Compared with two-layer mirror, our design provides a significant improvement of reflectance in 5–10 keV, and it also gives a good initial one for further optimization by other algorithms. Our job has a potential application in X ray astronomical imaging detection missions.

1. Introduction

In X ray region, refractive index of all materials is near to unity, and extinction coefficient is extremely small. Thus, X ray light will all transmit the materials with extremely small absorption and reflection. In X ray region, reflective optical system generally works in a grazing incidence mode by virtue of total reflection of materials. Generally, critical angle of total reflection is very small, and reflection decreases dramatically beyond this critical angle. The supermirror is often used to further increase reflectance beyond this angle. It is composed of alternative two materials with high- and low-density. Compared with metal substrate or two-layer mirror, it can provide better optical performance based on Bragg diffraction law in a broad wavelength or angular region [1–12].

Generally, three methods are used to design supermirrors, and they are Mezei method, Kozhevnikov method, and block method. Mezei method is also called as power-law method. The thickness distribution is derived by $d_i = a(b+i)^{-c}$, and d_{i} is bi-layer thickness, a and c are positive constants, b is a constant bigger than −1, i is the number of bi-layers [1,2]. In Kozhevnikov method, Kozhevnikov provided recurrent equations about the thickness of each layer in the multilayer based on analytical and numerical method. This method can give a good initial thickness distribution for complicated target reflectance curve, and it can save time for further refined optimization [3,4]. In block method, the multilayer is composed of several small periodic multilayers (blocks), each block has a specific period thickness (bi-layer thickness in a periodic multilayer), and it can reflect some specific wavelength based on Bragg diffraction law [5–7]. The supermirrors designed by Mezei and Kozhevnikov methods often have complicated thickness distribution, they require precise deposition velocity control, and even some small errors during deposition will result in severe optical performance deterioration. The supermirrors designed by block method have several sub-multilayers with different period thicknesses, and period thickness is easily to be controlled during fabrication and characterized. The shortcoming is that there are some oscillations in their reflectance curve [5–7]. The supermirrors used in NuSTAR [8] and ATHENA [9,10] were designed by Mezei method. The supermirror used in ASTRO-H [7] was designed by block method.

Supermirrors are widely used in synchrotron, plasma detection, astronomical imaging, biological microscopy [11], free electron laser. In this paper, we just focus on their space imaging application. W/Si supermirror was utilized in NuSTAR and X ray plasma imaging [12], and it has a good stability and optical performance in X ray region. To our knowledge, only W/Si supermirror with a grazing incidence angle of up to 0.7 degree was designed and fabricated [12]. Grazing incidence angle in X ray optical system is an important factor, and big angle can provide larger collecting area, shorter foci, less cost, and make alignment easier. In ATHENA, Ir/SiC and Ir/B_4C supermirrors were designed by Mezei method and fabricated, and the grazing incidence angle is up to 1.75 degree. However, they did not give a detailed description about their design. Here, we will design W/Si supermirrors with big grazing incidence angles of 1.0, 1.4, and 1.7 degrees in 0.2–10 keV based on block method

2. Design

In X ray region, complex refractive index of material is defined as Eq. (1), and δ is extremely small. Periodic multilayer is compose of two alternating materials with high (h)- and low (l)-density, and it can reflect a specific wave based on the Bragg diffraction law. Eq. (2) is a corrected Bragg formula [1], where m is diffraction order, d is period

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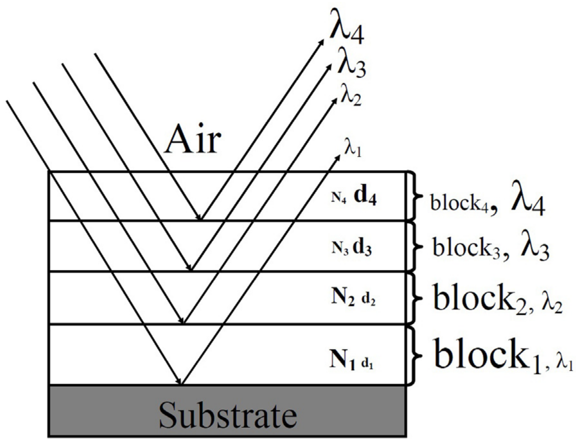

Fig. 1. The sketch for the principle of block method.

thickness, λ is the wavelength, Γ is thickness ratio of high-density material to a period d, θ is grazing incidence angle.

$$n = 1 - \delta - i\beta \tag{1}$$

$$m\lambda = 2d\sin\theta\left[1 - \frac{2\left(\Gamma\delta_h + (1-\Gamma)\,\delta_l\right)}{\sin^2\theta}\right]^{1/2} \tag{2}$$

Fig. 1 shows the sketch for the principle of block method. The supermirror is a combination of several periodic multilayers with different period thickness, each periodic multilayer is called as the block. Each block has N periods with a specific period thickness d, which is determined by Eq. (2). Since high-energy light can penetrate materials without significant absorption loss, we put the block_1 corresponding to high photon energy λ_1 near to the substrate. Then, block_2 corresponding to smaller photon energy λ_2 is stacked on the block_1. Such a procedure is iterated to the lowest target photon energy. That is to say, to reduce absorption, we set $\lambda_4 > \lambda_3 > \lambda_2 > \lambda_1$, and $d_4 > d_3 > d_2 > d_1$. Photon energy resolution is 0.02 keV. Thickness ratio Γ of high-density material to a period is set to be 0.5. W layer is put on Si layer in a period. Si layer is innermost one to be stacked on the substrate, and W layer is the outermost one, which is near to air. IMD software is used to calculate optical performance of supermirrors [13].

$$\tau \equiv R(\lambda)\exp\left[(4\pi\sigma\sin(\theta)/\lambda)^m\right]\exp(4\kappa_2(\lambda)z) \tag{3}$$

Our optimization strategy is listed as below:

(1) The period thickness at specific wavelength is determined by Eq. (2).

(2) Reflectance as a function of number of layer pairs at specific wavelength is calculated by IMD software, and the highest reflectance is obtained.

(3) Target reflectance of the supermirror at specific wavelength is one of key factors in the design. This factor is determined by Eq. (3) derived from Kozhevnikov method, and the details about this Equation can be found in Ref. [4]. Ref. [14] provided a detailed description about reflectance evaluation. Here, we do not give the derivation. This is different from classical block method, and they utilized integrated reflectivity to determine target reflectance [7]. According to Step (2), the required number of layer pairs for target reflectance at specific wavelength is also determined.

(4) By trial and error method, energy step between blocks is determined.

(5) Several blocks are stacked to compose a supermirror.

(6) Further optimization. The variable is thickness of each layer.

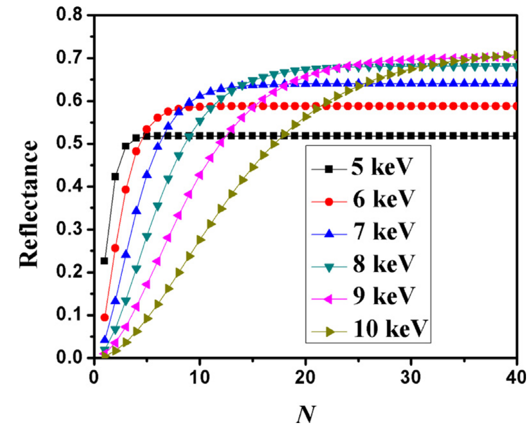

Fig. 2. Reflectance curves as a function of the number of layer pairs in 5–10 keV at 1.0 degree.

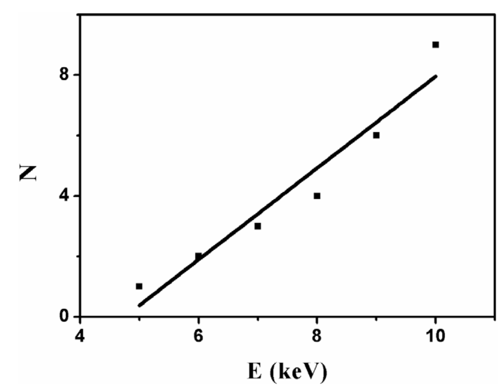

Fig. 3. The number of layer pairs as a function of the photon energy.

Table 1
Block structure in the design of 1.0 degree.

E (keV)	4	5	6	7	8	9	10
d (nm)	–	9.73	7.20	5.81	4.90	4.26	3.76
N	–	1	2	3	4	6	9

2.1. Design by block method

2.1.1. Design of 1.0 degree

Fig. 2 shows reflectance curves as a function of the number of layer pairs in 5–10 keV at 1.0 degree. For 5 keV, at first, with increasing of the number of layer pairs, the reflectance increases, and when the number of layer pairs is four, the reflectance is saturated. There is no increase in reflectance when more than four periods are added. With increasing of the photon energy, much more periods are required to yield saturated reflectance. Thus, $N_1 > N_2 > N_3 > N_4$. The saturated reflectance in 5 keV is the lowest, it increases with photon energy, and it is saturated in 8–10 keV. Target reflectance is evaluated by Kozhevnikov method, and it is set to be about 30% of saturated reflectance at 1.0 degree. Period thickness of each block is determined by Eq. (2). Table 1 gives block structure in the design of 1.0 degree. There are six blocks in this supermirror, they are corresponding to 5, 6, 7, 8, 9, and 10 keV, respectively, and they have corresponding period thickness and number of layer pairs. Period thickness ranges from 3.76 nm to 9.73 nm. The total thickness (Nd) of the block increases with the corresponding photon energy.

Energy step between blocks is another key factor in this design. Energy step should be slightly smaller than band width of reflectance zone of each block. Otherwise, a significant oscillation will occur in reflectance curve. Fig. 3 shows the number of layer pairs as a function

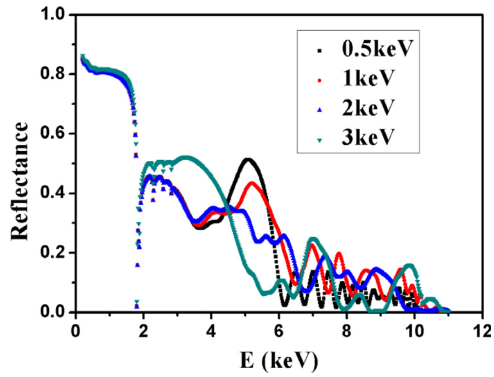

Fig. 4. Reflectance curves of supermirrors with energy steps of 0.5, 1.0, 2, 3 keV at 1.0 degree.

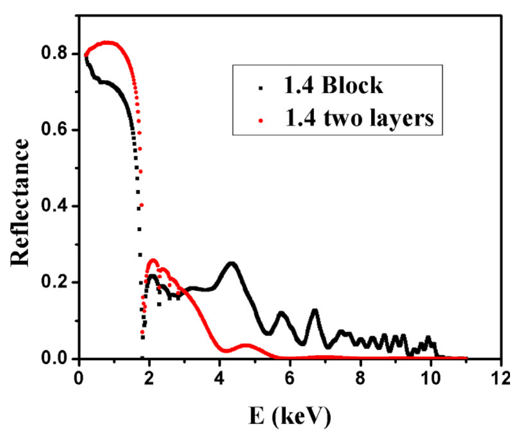

Fig. 5. Reflectance curve of the supermirror with an energy step of 1.0 keV at 1.4 degree.

Table 2
Block structure in the design of 1.4 degree.

E (keV)	4	5	6	7	8	9	10
d (nm)	7.99	5.82	4.63	3.87	3.33	2.93	2.61
N	1	2	3	5	7	10	15

of the photon energy. The number of layer pairs has a roughly linear relationship with the photon energy. To obtain broadband reflective mirror, reflectance zone of each block should be connected continuously. Thus, energy step should be carefully chosen. Fig. 4 shows reflectance curves of supermirrors with energy steps of 0.5, 1.0, 2, 3 keV. All the designs have significant oscillations in their reflectance curves, and design with an energy step of 1.0 keV has a better result. The average reflectance is 17.5% in 5–10 keV.

2.1.2. Design of 1.4 degree

Target reflectance at 1.4 degree is evaluated to be about 10% by Kozhevnikov method, and it is about 15% of saturated reflectance. As shown in Table 2, there are seven blocks in the supermirror working at 1.4 degree. Period thickness of seven blocks ranges from 2.61 nm to 7.99 nm in 4–10 keV. Reflectance curve of the supermirror at 1.4 degree is shown in Fig. 5. In this design, an energy step of 1.0 keV in 4–10 keV is selected. Significant oscillations occur in its reflectance curves. In 5–10 keV, the mean reflectance is about 6.0%. The mean reflectance of two-layer mirror (6 nm Si/10 nm W) is 0.3% in 5–10 keV, which is only one twentieth of our designed supermirror at 1.4 degree.

2.1.3. Design of 1.7 degree

Target reflectance is set to be 10% of saturated reflectance. Table 3 shows block structure in the design of 1.7 degree. There are seven

Table 3
Block structure in the design of 1.7 degree.

E (keV)	4	5	6	7	8	9	10
d (nm)	6.04	4.57	3.70	3.12	2.70	2.38	2.13
N	1	2	4	6	9	14	22

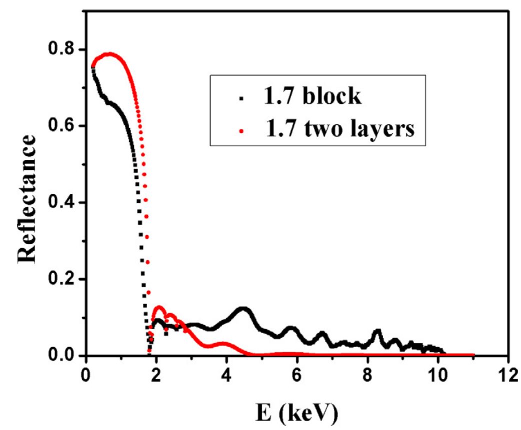

Fig. 6. Reflectance curve of supermirror with an energy step of 1.0 keV in 4–7 keV and 0.5 keV in 8–10 keV at 1.7 degree.

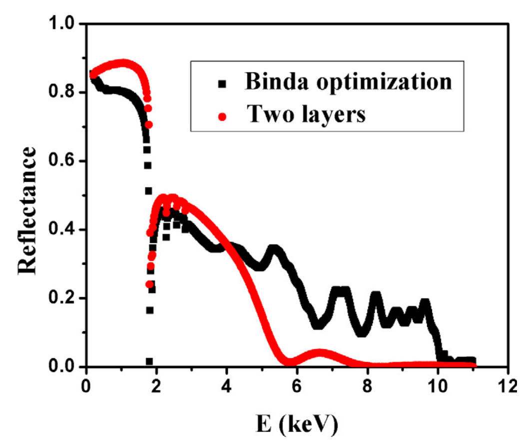

Fig. 7. Reflectance curve of the supermirror further optimized by Binda genetic algorithm at 1.0 degree.

blocks in this supermirror, and they are corresponding to 4, 5, 6, 7, 8, 9, and 10 keV, respectively. Period thickness ranges from 2.13 nm to 6.04 nm. Fig. 6 shows reflectance curve of the supermirror with an energy step of 1.0 keV in 4–7 kev and 0.5 keV in 8–10 keV. The design has significant oscillations in its reflectance curves. The average reflectance is 3.8% in 5–10 keV. For comparison, reflectance curve of two-layer mirror (6 nm Si/10 nm W) is also given. The average reflectance is 0.1% in 5–10 keV. Our design gives a supermirror with a high reflectance thirty eight times larger than two-layer mirror.

2.2. Refine optimization

The supermirror designed by block method can be further optimized by other optimization algorithms. Fig. 7 shows reflectance curve of the supermirror further optimized by Binda genetic algorithm [15] at 1.0 degree. The average reflectance is 18.7% in 5–10 keV. For comparison, reflectance curve of two-layer mirror (6 nm Si/10 nm W) is also provided. The average reflectance is 2.1% in 5–10 keV. Our supermirror provides a high reflectance nine times larger than two-layer mirror. Fig. 8 shows reflectance curve of the supermirror further optimized by Binda genetic algorithm at 1.4 degree. The average reflectance is

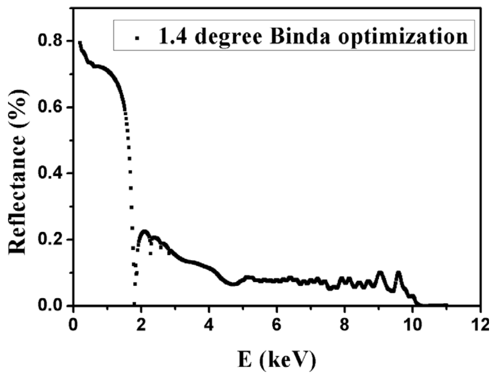

Fig. 8. Reflectance curve of the supermirror further optimized by Binda genetic algorithm at 1.4 degree.

7.0% in 5–10 keV. Binda genetic algorithm reduces oscillations in its curve, and makes a little improvement in reflectance. As shown in Fig. 6, the reflectance in 9–10 keV at 1.7 degree is low. We also do further optimization to solve this problem. However, as shown in Table 3, period thicknesses for 9.0 keV and 10 keV block are 2.38 nm and 2.13 nm, respectively. The minimum period thickness is set to be 2.0 nm in our design due to physical available thickness limit. Period thickness that can be chosen is less during further optimization at 1.7 degree. Thus, unfortunately, no better design is obtained for 1.7 degree after further optimization.

3. Conclusion

W/Si supermirrors are designed by block method. The big grazing incidence angles are 1.0, 1.4, and 1.7 degrees, respectively. The photon energy ranges from 0.2 to 10 keV. The average reflectances are 18.7% in 5–10 keV at 1.0 degree, 7.0 at 1.4 degree, and 3.8% at 1.7 degree, respectively. Compared with two-layer mirror, a significant reflectance enhancement of up to thirty eight times is achieved. There are two innovations in our paper. First, our designed mirrors has a big grazing incidence angle of up to 1.7 degree. Second, target reflectance is evaluated by Kozhevnikov method, and, according to target reflectance at specific block, the required number of layer pairs is determined. The ratio of target reflectance to saturated one is not fixed for different incident angles. Our strategy is different from Ref. [7]. They chose target reflectance equal to 60% of the saturated one. Because these designs do not require precise deposition rate control, they can be fabricated easily. Our job has a promising application in X ray imaging system.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Xiaodong Wang: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Writing - original draft. **Bo Chen:** Supervision. **Haifeng Wang:** Software. **Li Zhang:** Writing - reviewing & editing. **Shuai Ren:** Writing - reviewing & editing. **Peng Zhou:** Writing - reviewing & editing.

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