15

Project of a two-mirror monochromator for the photon energy range 8-36 keV for the "SKIF" synchrotron

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A project of an X-ray monochromator for the "SKIF" synchrotron based on two flat mirrors with multilayer reflective coatings is reported. The concept of the monochromator is based on the absence of precision mechanical systems and feedthroughs in vacuum, which significantly reduces mirror surface contamination and increases scanning accuracy. In addition, the overall structure of the device is greatly simplified in this way, which in turn leads to a significant reduction in the total cost and labor for manufacturing. The grazing angle of incidence of radiation on the mirrors in the process of scanning by photon energy varies within $0.5-1.3^{\circ}$. The length of the mirrors is 120 mm, the assumed size of the input beam is $1 \times 1 \text{ mm}^2$. A wide operating energy range, 8-36 keV, is achieved through the use of 3 strip-mirrors with coatings of different chemical composition, namely: Mo/B4C, W/B4C and Cr/Be. The article presents the X-ray optical scheme, the expected reflection coefficients and spectral selectivity of the monochromator, the results of the calculation of thermally induced surface deformations and the corresponding slope errors of the first mirror.

Keywords: synchrotron radiation, multilayer mirror, monochromator, surface.

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Introduction

Due to moderate spectral selectivity ($\Delta\lambda/\lambda \sim 1\%$), high (of the order of 60–90%) reflection coefficients, large geometric dimensions and the possibility of creating gradient reflective coatings multilayer X-ray mirrors (MXRM) are widely used in modern scientific, technical and technological equipment. Compared to crystals, MXRM-based monochromators increase the radiation intensity up to two orders of magnitude, which makes them extremely promising for X-ray microscopy, lithography and a number of other applications where it is required to collect as many photons as possible [1–3].

In the conditions of synchrotrons of the 3rd and 4th generations, as well as X-ray free electron lasers, in some cases MXRM allow switching from cryogenic to water cooling of the working reflective elements of the corresponding monochromators, since due to the smaller angles of incidence, the power density of incident radiation on the surface of the MXRM is more than an order of magnitude less than on crystal [4,5].

The synchrotron radiation source (SI) of the 4th generation "SKIF" [6] currently being developed at the INP SB RAS is also planned to use MXRM for various applications. In particular, at the experimental Station 1-1, Microfocus" a two-mirror monochromator with a tunable X-ray wavelength is supposed to be used for SI monochromatization.

This paper describes the two-mirror monochromator proposed by the authors, the principles of its design and the main technical characteristics.

1. Requirements for monochromator and Device principles

According to the scientific program and technical specification, a two-mirror monochromator must meet the following requirements:

— the operating range of photon energies is 8-36 keV, divided into sub-bands:

- "soft" energy 8-14 keV;
- "main" 14–36 keV;
- "hard, high resolution" 30-36 keV;

— spectral selectivity in "soff" and "basic" ranges $\Delta\lambda/\lambda \sim 0.7-1$ %, and $\Delta\lambda/\lambda < 0.5$ % in "hard, high resolution";

— MXRM reflection coefficients > 60%;



Figure 1. A design diagram indicating the basic geometric characteristics of a monochromator for two energy limits: minimum (top) 8 keV, and maximum (bottom) 36 keV.

— the captured size of the synchrotron beam at all energies $\leq 1 \times 1 \, \text{mm}^2;$

- range of working angles MXRM 0.5–1.3°;
- X-ray power absorbed by the first mirror 20 W;

— permissible thermally induced wavefront distortions after the first mirror $< 1.7 \,\mu$ rad;

- mirror cooling: water;

— displacement of the axes of the incident and reflected beams by the second mirror (offset — difference between the positions of the beams in space) ≥ 10 mm.

The choice of the maximum working angle value in 1.3° will be discussed below. From the geometric dimensions of the beam and the working angles, it is not difficult to determine that the length of the mirrors should be at least 115 mm. In the project, the length of the mirrors is chosen to be 120 mm.

The design diagram of a monochromator with basic geometric characteristics for offset in 16 mm is shown in Fig. 1. The upper part of the figure corresponds to the setting for the minimum, and the lower one for the maximum photon energy.

The monochromator is based on the following fundamental concept. To ensure a constant position and direction of the monochromatic beam at the output of the monochromator for any energy, two identical MXRM parameters are used. Since in the process of energy scanning, the beam reflected from the first mirror changes direction in accordance with the Bragg condition, the second mirror, in addition to adjusting the Bragg angle, performs linear displacement so that the beam reflected from the first mirror accurately hits the center of the second mirror. In this case, the beam coming out of the monochromator will retain both the direction of movement, parallel to the beam entering the monochromator, and a constant shift in space (offset), almost regardless of the working energy.

Traditionally, monochromators of this type, for example [7], are designed and built in such a way that all highprecision mirror drives (tilts, turns, linear movements) are located in a single vacuum chamber. This design of the monochromator has a number of disadvantages. Firstly, in the case of a wide operating wavelength range, for example, in our case, the vacuum chamber will have large (more than 1.05m) dimensions. This leads to two negative consequences. Firstly, to ensure an ultra-high at the level of 10^{-9} Torr vacuum requires very powerful pumping means. Secondly, atmospheric pressure leads to severe deformations of the chamber, which can negatively affect the accuracy of alignment. Thirdly, the presence of a large number of drives in vacuum negatively affects the contamination of mirrors with decomposition products of hydrocarbons, which are necessarily present in the insulation of wires and lubrication. Fourthly, expensive and, as a rule, less reliable electromechanical components have to be used to minimize contamination.

The novelty of our concept is the use of relatively small vacuum chambers and the removal of all critical precision movements from the vacuum outside into the atmosphere. The device uses three small vacuum chambers with a diameter of about 150 mm. The first (on the left in the course of the incident beam) and the last cameras remain stationary in the direction of the optical axis of the device, and the second moves widely. Mirrors are installed in the first and second cameras. The first camera is mounted on a system of movements that provide the following types of movements for alignment and energy scanning:

— transverse (perpendicular to the direction of propagation of the X-ray beam) within ± 10 mm with step 5 μ m; — vertical movement within $\pm 10 \text{ mm}$ with increments of $10 \,\mu\text{m}$;

— rotate the mirror to set the Bragg angle within $\pm 2^\circ$ with increments of $0.0002^\circ.$

Vertical movement is caused not only by the precision adjustment of the monochromator to the synchrotron beam, but also allows you to quickly change the type of multilayer coating in the presence of several strips with MXRM on the same substrate.

The system of movements of the second camera, in addition to those noted above, includes a goniometer to control the inclination of the plane of the second mirror in relation to the first and a long linear movement for scanning by energy. The goniometer provides a slope in the range of $\pm 2^{\circ}$ in increments of 0.001° . The longitudinal, linear movement provides movement in the range of $\approx 1 \text{ m}$ with 0.05 mm increments.

To ensure the required kinematics of the device, the central chamber is connected to the stationary chambers by means of a welded bellows, which provides a range of movements of about 4 times with respect to the compressed state. The device will be mounted on a thick dimensionally stable granite slab. Pre-pumping will be carried out by dry pre-vacuum and turbomolecular pumps with the possibility of their subsequent disconnection from the device. The ultra-high vacuum will be maintained by magnetic discharge pumps with a capacity of 25 l/s installed on the first and last vacuum chambers.

2. Thermal calculations

Taking into account the high intensities of the SI beams, one, among others, an important circumstance/factor limiting the maximum operating angle of multilayer mirrors is the absorbed power per unit area of the mirror, leading to thermally induced deformation of the surface and, accordingly, the reflected wavefront. Thermal calculations were carried out to solve this problem. The mirror was a silicon substrate 120 mm long, 15mm high and 50mm thick. Cooling from the top and bottom of the first mirror was carried out with water at a temperature of 25° C through copper radiators pressed against the upper and lower faces, through indium gaskets 0.2mm thick. Fig. 2, a explains the cooling scheme. Fig. 2, b, c shows the temperature field and the deformation of the surface at grazing incidence of radiation on the mirror 1.5° , beam size $1 \times 1 \text{ mm}^2$ and SI power 20 W. Fig. 3 shows the temperature, strain, and angular error profiles along the mirror in the central part of the beam trace. For clarity, local angular errors expressed in μ rad, in Fig. 3 increased by 10 times. That is, the value of $1\,\mu$ rad on the graph corresponds to an error of $1.5\,\mu$ rad. Since for the angle of incidence 1.5° the beam trace on the mirror is ± 19 mm, the maximum angular error is about 1.6 μ rad. This is comparable to the requirements of the technical specification for the device. Therefore, to ensure a margin when designing the device, the maximum angle



Figure 2. Cooling system of the first mirror (*a*), temperature field (*b*) and surface deformation (*c*) at a grazing incidence of radiation on the mirror 1.5° , beam size $1 \times 1 \text{ mm}^2$ and power SI 20 W.



Figure 3. Deformation profiles (1), thermally induced local errors (2) and temperature field (3), mirror surface shapes corresponding to the conditions given in Fig. 2.



Figure 4. Spectral dependences of the expected reflection coefficients (R^2) and selectivity ($\Delta E/E$) at the output of the monochromator, taking into account the identity of mirrors and double reflection. MXRM Mo/B4C: N = 120, d = 3.71 nm, $\beta = 0.25$, $\sigma = 0.4$ nm.



Figure 5. Spectral dependences of the expected reflection coefficients and selectivity at the output of the monochromator, taking into account the identity of mirrors and double reflection. MPS W/B4C: N = 200, d = 2.0 nm, $\beta = 0.33$, $\sigma = 0.3$ nm.

was taken 1.3° . The minimum angle was determined for reasons of capturing the entire SI beam and minimizing the size of the mirrors, and was 0.5° .

3. Selection of types of multilayer X-ray mirrors

The main criteria for choosing the composition and design of multilayer X-ray mirrors are reflection coefficients and spectral resolution in the operating range. Optimal materials were selected for each wavelength range, taking into account the working angles. So, for the photon energy range 8-14 keV, a pair of Mo/B4C materials with the following characteristics was selected: the number of periods N = 120, period d = 3.71 nm, the proportion of molybdenum in the period $\beta = 0.25$, interlayer roughness $\sigma = 0.4 \text{ nm}$. To cover the entire energy range, the grazing

incidence of SI on the mirror varies within $\theta = 0.65 - 1.23^{\circ}$. Fig. 4 shows the spectral dependences of the expected reflection coefficients and selectivity at the output of the monochromator, taking into account the identity of the mirrors and double reflection. As can be seen from the figure, the reflection efficiency of the monochromator exceeds 70% in the entire operating wavelength range, however, the spectral selectivity is approximately 1.5 times higher than required. To solve this problem, at the stage of mirror manufacturing, it is planned to achieve the required spectral bandwidth of 1% by optimizing the parameter β . If, with a decrease of β , a strong drop in the reflection coefficient is observed, then, as an alternative, the V/B4C pair will be studied, which, on the contrary, is characterized by a relatively high spectral selectivity at the level of 0.8%. At the same time, the reflection coefficient V/B4C with double reflection in the operating range varies within 45-80%.



Figure 6. Spectral dependences of the expected reflection coefficients and selectivity at the output of the monochromator, taking into account the identity of mirrors and double reflection. MXRM Cr/Be (blue thin lines (in online version)) and Cr/B4C (red thick (in online version)): N = 500, d = 2.0 nm, $\beta = 0.5$, $\sigma = 0.43$ nm.

For "of the main" range 14–36 keV, as in most works, see for example [8], the W/B4C structure with parameters is selected: N = 200, d = 2.0 nm, $\beta = 0.33$, $\sigma = 0.3$ nm. According to data [9] when using an RF magnetron discharge on a W-target, the length of the transition region can be reduced to $\sigma = 0.24$ nm. Thus, the result of calculating the reflection coefficient shown in Fig. 5 can be considered a lower estimate. It can also be seen from the figure that this pair of materials satisfies the requirement for a spectral bandwidth at the level of 1%.

For the so-called "hard, high resolution" subrange, the photon energy range is 30-36 keV, a better spectral resolution is required 0.5%. When choosing the most effective pair of materials for this range, MXRM consisting of relatively light materials were analyzed. Among the most promising systems were Cr/Be, Cr/B4C. In the literature for short-period MXRM, we found data on the length of transition regions only for Cr/Be [10] and which was In the study [1], the Cr/B4C pair was $\sigma = 0.43$ nm. discussed, but no data on the length of the transition Therefore, calculations for both regions were given. systems were made for the following parameters: N = 500, $d = 2.0 \,\mathrm{nm}, \ \beta = 0.5, \ \sigma = 0.43 \,\mathrm{nm}.$ Fig. 6 shows the results of recalculation. Blue thin lines (in online version) correspond to Cr/Be and thick red (in online version) -Cr/B4C.

The following main conclusions can be drawn from Fig. 6. Firstly, both structures meet the requirements of the technical specification both in terms of reflection coefficient and spectral selectivity. The spectral resolution was 0.3%. Secondly, the "mode of increased resolution" is observed not only in the area of 30-36 keV, but also in a wider (14-36 keV) range. Thirdly, with the value of the interlayer transition region 0.43 nm, which was found in Cr/Be MXRM, they look more preferable compared to Cr/B4C. However, the final choice in favor of one or another

pair of materials will be made based on the results of structural and reflectometric measurements of real short-period Cr/B4C MXRM.

Conclusion

A project of a monochromator with tunable working energy of photons in the range of 8-36 kav has been developed. Two flat multilayer mirrors with identical reflective characteristics act as dispersing elements. The monochromator provides the required quality level of the reflected front, the angular error is less than 1μ rad at the output when the power incident on the first mirror is up to 20 W. The entire range of working photon energies is divided into three sub-bands. Each sub-band has its own pair of multilayer mirrors. The adjustment to the subrange is carried out by vertical displacement of both mirrors. To do this, three identical strips are formed on each mirror in pairs. Materials are selected for the first two sub-ranges: Mo/B4C and W/B4C. For the third, high-resolution subrange, two promising pairs of materials Cr/Be and Cr/B4C were selected and analyzed. The final choice has not been made, since there are no data in the literature on transition layers in short-period Cr/B4C MXRM. Structural and reflectometric studies of this pair of materials are planned in the near future. With equal values of the transition region, the Cr/Be system looks more preferable.

The paper describes the basic device and design features of the device. It is assumed that such a device will be implemented and installed on the synchrotron "SKIF" as part of the first stage of development of experimental stations.

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Conflict of interest

The authors declare that they have no conflict of interest.

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