GRADED d-SPACING MULTILAYER OPTICS FOR VARIOUS ENERGIES

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ABSTRACT

Graded d-spacing multilayer optics for Mo Kα, Co Kα and Cr Kα have been developed. Using Monte-Carlo ray tracing methods, the authors have studied many aspects involved in multilayer optic design. These include the dependence of multilayer performance on source intensity distribution, coating material choice, multilayer configuration and optical layout. In addition, the influence of coating and curvature errors are addressed. Performance is also studied experimentally and compared to the theoretical results. In addition to the study of single multilayer optical system, the performance a multilayer's system combined with a channel-cut crystal is also discussed.

OPTIMIZATION BY USING Monte-Carlo RAY TRACING METHOD

The performance of multilayer optics depends on many factors including the optical layout, multilayer characteristics, x-ray source characteristics and specific applications [1]. Important performance parameters include flux, beam width, Kβ reduction and divergence. Evaluation by analytical calculation is difficult due to the complex nature of the systems. The calculation often involves multifold integration in which the integrand is very difficult to define, and sometimes even impossible to define by an analytical function. Although some quantitative characteristics can be predicted with geometrical modeling, the results tend to be coarse and, sometimes, even incorrect. One alternative method is Monte-Carlo ray tracing method, which changes an integration problem into a summation of a series of simple events. With the calculation power of modern PCs, the evaluation with Monte-Carlo method can be done in a matter of a few minutes. The detailed description of Monte Carlo method applied to the evaluation of multilayer optics is provided in another paper [2] and the following is some of the major points.

The parameter describing flux is "efficiency", defined as the probability of an isotropically emitted photon being reflected and passing through slits, if there are any. The efficiency is given by formula (1), where \( R_{\alpha} \) represents the reflectivity for \( K_\alpha \) and \( \Delta \theta_i \) is the capture angle opened by the mirror at a specific source point \( x_i \); \( T_i \) is the transmission function of the slits whose value is either 1 for the transmitted or 0 for the blocked photons; and \( N \) is the number of "events" used in the calculation.

\[
\epsilon_\alpha = \frac{1}{2\pi N} \sum_i R_{\alpha} \Delta \theta_i T_i
\]  

(1)

The efficiency of \( K_\beta \) can be calculated by the same formula by replacing the \( K_\alpha \) reflectivity with the respective \( K_\beta \) reflectivity. Therefore, the \( K_\beta / K_\alpha \) ratio can be obtained simply by
where \( c \) is the intensity ratio of \( K_{\alpha} \) and \( K_{\beta} \) in the incident beam. Other performance parameters, such as the beam profiles and beam widths at various positions can be found out by tracing each ray or "photon" and registering them at these locations.

**SOURCE MODEL AND MULTILAYER CHARACTERISTICS**

The deviation from strict focusing or collimating is directly associated with the source intensity distribution. Moreover, the finite rocking curve of a multilayer yields a limited view angle to the source, resulting in an insufficient usage of the source and therefore low flux. Two source models simulated by a random generator [2] have been used for the simulations. One has a single peak, which is a good approximation for a rotating anode and some sealed tubes. The other one has double peaks and has been found experimentally from some sealed tubes, which is caused by the projection of the tube’s coil-shaped filament. In this study, a typical sealed tube configuration is used, which is 40 micrometers at a 6 degree take-off angle and a power loading of 2.0 kW.

Some multilayer material combinations are considered. Figure 1 shows the peak reflectivity and FWHM for Mo K\( \alpha \), Co K\( \alpha \) and Cr K\( \alpha \).

![Figure 1. Peak reflectivity and FWHM for different material combinations](image-url)
Generally speaking, the shorter the wavelength of the x-rays, the narrower the rocking curve of a multilayer used for the x-rays. This is because x-rays with shorter wavelength have lower absorption and more layers are involved in the diffraction. As \( \text{K}\beta \) is very close to \( \text{K}\alpha \) for each element, the multilayer performance for \( \text{K}\beta \) can be considered as the same for \( \text{K}\alpha \). Different material systems, such as \( \text{W/B}_4\text{C} \), \( \text{Mo/B}_4\text{C} \), \( \text{Ni/B}_4\text{C} \) and \( \text{Ni/C} \), can be considered for multilayer coating. Since second order suppression is generally required, all of the multilayer coatings considered in this study have a \( \gamma \), the thickness ratio of heavy sub-layer and light sub-layer, equal to 50%. The characteristics of multilayers are different for different wavelengths. In ray tracing calculation, these parameters, as the source intensity distribution and optical layout, are the system parameters.

**PERFORMANCE EVALUATION FOR Mo K\alpha, Co K\alpha AND Cr K\alpha**

Parabolic mirrors have been studied in this paper. The source-mirror distance is chosen as 100 mm to allow enough room for hardware implementation. The dimension of most sealed tubes is about 80 mm, allowing a space of 30 mm between the source and the mirror. The simulation study shows flux would not significantly increase by using a shorter source-mirror distance since the "source usage efficiency" decreases at a closer distance. The source usage efficiency is defined by the throughput with the real source divided by the throughput with a point source. The mirror length is chosen to be 60 mm, which will given enough beam width for most applications. Considering the trade-off between capture angle and peak reflectivity, center d-spacing is chosen as 35 angstroms and d-spacing range is 29.28 to 39.90 angstroms. The study shows [3] that the influence of refraction to d-spacing is independent from wavelength and d-spacing defined by Bragg's law could be maintained if proper geometric parameters are chosen. Therefore, the same multilayer can be used for different wavelengths, although flux and divergence of the reflected beam determines the choice of the coating. Some performance parameters obtained from the simulation study are shown in Figure 2.

![Figure 2. Source usage efficiency, efficiency and K\beta/K\alpha ratio](image-url)
One major issue in the optical design is that the rocking curve must match with the source width to achieve maximum flux. From Figure 2, one can see that the FWHM of the rocking curve decreases greatly for Mo Kα for all the material combinations. The narrow rocking curve results in poor source usage efficiency and the small Bragg angle yields a small capture angle. The convolution of these two yields low overall efficiency. On the other hand, rocking curve width is not a primary issue for Co Kα and Cr Kα; peak reflectivity plays a more important role. Therefore, Ni/B₄C is the preferred coating for Co Kα and Cr Kα. Other than total flux, angular distribution of the reflected beam is also important for some applications. The beam divergence is determined by the source size and the multilayer rocking curve. Figure 3 shows the angular distribution of the reflected beams, normalized to the same number of incident photons.

Figure 3. Angular distribution of the reflected beams

W/B₄C and Mo/B₄C are the better choices for Mo Kα. W/B₄C provides the widest rocking curve, therefore the best source usage efficiency, resulting in the highest flux. Mo/B₄C has a very high reflectivity and narrow rocking curve. Therefore, the Kβ reduction is better and divergence is smaller. For some high resolution applications, for example coupled with a channel-cut monochromator, the performance with Mo/B₄C coating is better due to its higher peak value. For Co Kα and Cr Kα, the best performance comes from Ni/B₄C coating. Ni/B₄C offers the highest flux, good Kβ reduction and the smallest divergence.

Effect of d-spacing inaccuracy and figure error

Study has shown that the d-spacing inaccuracy, the deviation of the layer thickness from theoretical value, and optical figure error, the curvature deviation from theoretical value, reduce the peak value of the angular distribution and cause uniformity problems. In general, these errors, especially figure error, do not cost much in total flux. Figure 4 shows the effects on a Co Kα mirror with Ni/B₄C coating as an example. The Total flux loss is less than 3% for the figure error. However, the peak height of the angular distribution is lower by about 10%. If the mirror is coupled to a channel-cut monochromator, the total through-put of the system will drop by
about the same mount. Uniformity is much worse than the case without errors.

Figure 4. Influence of d-spacing error and figure error

Osmic's current coating and precision optical construction technology has reduced the d-spacing inaccuracy to an average value of 0.1 angstrom, and figure error to an average of 0.1 arc minutes. The best achieved accuracy is 0.08 angstroms for d-spacing error and 0.05 arc minutes for figure error. These have improved the beam uniformity substantially.

MIRROR FABRICATION AND PERFORMANCE EVALUATION

Optics for Mo Kα, Co Kα and Cr Kα have been constructed and tested. For evaluating the efficiency of the optics, a parameter called throughput defined by the output flux divided by the incident flux, is measured for each mirror. Theoretical values converted from "efficiency" then are used to make comparisons. Figure 5 shows a good agreement between the theoretical and measured value. Also shown on Figure 5 is the beam uniformity and beam profile of Co mirror after channel cut crystal, measured 300 mm from the source.

Figure 5. Throughput and beam profiles
Figure 6 shows the spectrums measured by a EDS detector. The data are normalized to the Kα peak. The Kβ reduction is about 40 times for Mo, 270 times for Co and 290 times for Cr.

![Figure 6. Spectrum measurement](image)

Angular scan is done by using a single crystal (Si) analyzer and the measurement result for Mo is given in Figure 7. The measured FWHM is 2.0 arc minutes.

![Figure 7. Angular scan with Si (111) for Mo mirror](image)

**SUMMARY**

A much better understanding of the performance of multilayer optics has been obtained by using Monte-Carlo simulation study. Performances includes many aspects such as dependence of coating selection, influence of d-spacing and figure errors, angular distribution of the reflected beam, system efficiency and Kβ reduction. Based on the simulation study, optics for Mo Kα, Co Kα and Cr Kα have been designed, fabricated and tested. A good agreement is reached between measurement result and theoretical expectation.

[3] Verman, B. and Jiang, L., to be published