

## **Design of a multilayer grating for the soft X-ray tomography beamline**

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### **Abstract**

The soft X-ray tomography (SXT) beamline using a bending-magnet source is designed for transmission full-field imaging of frozen-hydrated biological samples in the range between 260 eV and 2600 eV. In this beamline, the plane-grating monochromator (PGM) consists of two interchangeable plane gratings and a plane mirror to provide uniform energy-independent illumination. Now the 600 l/mm grating with Au coating has already been set up to serve the energy range from 260 eV to 1200 eV. Here a multilayer coating on the surface of the 2400 l/mm grating will be study for enhancing the diffraction efficiency in the energy range from 1200 eV to 2600 eV.

The soft X-ray tomography (SXT) beamline using a bending-magnet source is designed for transmission full-field imaging of frozen-hydrated biological samples in the range between 260 and 2600 eV [1]. Figure 1 shows the schematic layout of the SXT beamline with the varied-line-spacing plane-grating monochromator (VLS-PGM). The monochromator consists of two interchangeable VLS plane gratings and a plane mirror to provide uniform energy-independent illumination. Now the 600 l/mm grating with Au coating has already been set up to serve the energy range from 260 eV to 1200 eV. Here the 2400 l/mm grating with the multilayer coated will be used to cover the energy range from 1200 to 2600 eV. In the PGM, the alternate multilayer (AML) grating should be paired with a mirror coated with a similar multilayer which compensates the grating deviation [2]. Here the computer program called IMD is used to calculate the reflectance of multilayer films [3]. The relations between the grazing incidence angles and the reflectance for the AML PM could be calculated by IMD, as shown in figure 2. The figure 3 shows an ideal model of the alternate multilayer grating. We consider that the Mo<sub>2</sub>C/B<sub>4</sub>C alternate layers of two materials are deposited on a lamellar grating substrate. The groove depth of  $d$  is 2.5 mm, the period of multilayer film is 30 and its duty cycle is 0.5. The AML grating should provide a high-efficiency for the first diffraction order, and the  $k = 1$  will be used. The grazing angles with high reflectance for the PM could be used to find out the grazing incidence angle for the AML grating from solving the grating equation, as shown in figure 4. For VLS plane grating, the parameters of groove density can be expressed by:

$$N = dn / dw = N_0 (1 + a_1 w + a_2 w^2 + a_3 w^3 + \dots)$$

in which  $w$  is the position on the grating along the light propagation direction,  $N$  is the groove density,  $N_0$  is the groove density at the center of the grating and  $a_i$  are space variation parameters. The optimization principle and process are described in detail in some literatures [2,3]. The space variation parameters of gratings were optimized to reduce the effect of defocus, coma and spherical aberration and keep the exit slit in focus for any value of incident angle. For 2400 l/mm AML grating optimized at 2473 eV, the parameters of  $a_1$ ,  $a_2$ , and  $a_3$  are  $-7.49 \text{ mm}^{-1}$ ,  $1.2 \times 10^{-2} \text{ mm}^{-2}$ , and  $-1.61 \times 10^{-5} \text{ mm}^{-3}$  respectively. In this study all optical parameters are verified with the ray tracing method.

The basic idea is to alternate layers of two materials in order to synthesize a 2D periodic structure in the plane perpendicular to the grating lines. The AML grating has properties similar to crystals used in high energy double crystal monochromator, namely only waves satisfying a Bragg condition are reflected. This enhances the diffraction efficiency in the allowed orders.

the black lines describe the relationship between photon energy and grazing angle of incidence. The blue lines describe the relationship between photon energy and beam position on the plane mirror.

For 2400 l/mm grating optimized at 2400 eV, the parameters of  $a_1$ ,  $a_2$ , and  $a_3$  are  $1.00 \times 10^{-16} \text{ mm}^{-1}$ ,  $-5.92 \times 10^{-7} \text{ mm}^{-2}$ , and  $-9.45 \times 10^{-10} \text{ mm}^{-3}$  respectively. In this study all optical parameters are verified with the ray tracing method. In figure 2, the black lines describe the relationship between photon energy and grazing angle of incidence. The blue lines describe the relationship between photon energy and beam position on the plane mirror. The calculated resolving power and flux at the exit slit are shown in Fig. 3 and Fig. 4, respectively.