Small-offset Virtual Channel-cut Monochromator for Sub-micron X-ray Diffraction Beamline at Taiwan Photon Source

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Abstract. In this report, we illustrate the design concept of the small-offset(1 mm) virtual channel-cut monochromator. The monochromator is specially designed for Sub-micron X-ray Diffraction Beamline at Taiwan Photon Source. It can offer a monochromatic beam with the resolving power better than 5000 in the range of 7 keV–25 keV and allows the beamline to cycle between the polychromatic and monochromatic modes with a fixed spot of 100 nm at the sample position. Its adjustments and the thermal deformation are reduced as possible to increase the stability of the focal point. The finite element analysis of the thermal deformation shows rather simple cooling techniques can be used. Base on above design, we expect the positional stability of the focus can be kept in around 10 nm.

1. Introduction

The Taiwan Photon Source (TPS) is a new 3 GeV low-emittance synchrotron storage ring at National Synchrotron Radiation Research Center, Hsinchu, Taiwan. Thanks to its low-emittance(1.6 nm – rad), a new opportunity has been created to map the mesoscale structure and dynamics with sub-micron resolution[1, 2]. Sub-micron X-ray Diffraction Beamline is one of the initial phase beamlines at TPS and will be open to the academic and scientific communities in the middle of 2015. This beamline is aimed to observe 2D/3D images based on hard X-ray Laue/Bragg diffraction techniques with sub-micron resolution for materials science research. In this report, we describe the design of the small-offset virtual channel-cut monochromator for this beamline.

2. Optical layout of the beamline

The optical layout is in figure 1. The source is a 3 m-long undulator with 137 periods and the maximum magnetic field is 1.05 T. Its gap can be tapered 2 mm to produce a polychromatic beam for Laue diffraction[3]. Because the horizontal source size of 288 μm(FWHM) is too large for a 100 nm focusing, a defining slit at 25 m is used to reduce the beam width. The energy of the monochromatic beam can be selected by the monochromator at 62 m. The polychromatic beam comes from the vertically off-axis part of the radiation. At 61 m, a selecting aperture with
120 µm × 450 µm (H × V) opening allows one of the two beams to pass through at a time. In order to focus the polychromatic beam, an achromatic Kirkpatrick-Baez mirror pair[4] is adopted and images the source to a 100 nm spot at the sample position. Considering the de-magnification and the working distance, the vertical and the horizontal focusing mirrors are placed at 68.83 m and 68.95 m respectively. Their grazing angles are 3.0 mrad and useful lengths are 150 mm and 40 mm respectively. The coatings are 600 Å Pt with the surface roughness of 1 Å.

![Figure 1. Optical layout of BL21A Sub-micron X-ray Diffraction Beamline at TPS.](image)

3. Design of the monochromator

3.1. Position, heat load, acceptance and cooling

In order to increase the stability of the focal point, the thermal deformation of the monochromator should be reduced as possible. Due to the focusing system only accepts a small fraction of the source radiation, the useful acceptance of the monochromator is limited by 120 µm × 450 µm (H × V). Under such a condition, the incoming power is 0.65 W and the peak power density is 16.9 W/mm² when the ring current is 0.5 A. We have analyzed the positional dependency of the thermal deformation[5, 6]. The normalized thermal deformation is 1, 0.125 and 0.0156 for the monochromator is placed at 30 m, 60 m and 120 m respectively. Obviously, placing the monochromator far away from the source can effectively reduce the thermal deformation. Considering the beamline arrangement and the thermal deformation, the monochromator is placed at 62 m from the source.

We also performed the simulation of the thermal deformation by the finite element analysis for different cooling schemes. The results for the simple side cooling are summarized in table 1. The crystal dimension is supposed to be 20 mm × 20 mm × 20 mm (L × W × H). At the minimum working energy of 7 keV, the slope error of the first crystal is 0.12 µrad and the vertical spot size increases less than 10 nm when the cryogenic cooling is applied. For the watering cooling, the slope error is 0.69 µrad. The vertical spot size increases to 151 nm due to the cylindrical shape of the thermal deformation. It is possible to compensate the thermal deformation by slightly tuning the grazing angle of the vertical focusing mirror. Thus, the simple water-cooling is also applicable for this beamline.

3.2. Crystal, offset and overlap

This beamline will be operated in the energy range of 7 keV–25 keV and the requirement of the resolving power is better than 5000. Si(111) is used as the diffraction plane because Si crystal
Table 1. Brief summary of the finite element analysis and ray-tracing at the energy of 7 keV. ∆ is the slope error. $I_0$ is the normalized monochromatic flux at the sample position. $\Delta E$ is the bandpass of the monochromator.

| Cooling Type     | $\Delta$ (rms) (µrad) | Spot size (nm$^2$) | $I_0$ | $\Delta E$ (eV) |
|------------------|------------------------|--------------------|-------|-----------------|
| ideal            | 0                      | $52 \times 62$    | 1     | 0.79            |
| Water-cooling    | 0.69                   | $50 \times 151$   | 0.91  | 0.78            |
| Cryogenic cooling| 0.12                   | $52 \times 70$    | 0.96  | 0.78            |

has a good quality and its properties are well studied.

The beam offset is determined by three considerations. In order to fix the position of the focus when the beamline is cycled between the polychromatic and the monochromatic beams, it is necessary to slightly tune the outgoing angle of the diffraction beam for making the two beams coincident. The fine tune of the diffraction angle can be achieved by heating the crystal, mechanically tuning and acoustically tuning[7, 8]. In this design, the mechanically tuning is adopted because of its convenience and good stability. The mechanically tuning is to slightly detune the Bragg angle of the second crystal. The angular deviation between the two crystals must be smaller than the Darwin width at the highest working energy, or the output flux will drops severely. That is the first consideration for the beam offset. Secondly, the polychromatic flux decreases in the radial direction(See figure 2). Finally, we can use a long crystal to avoid moving the crystal along the crystal surface(Y direction). The required crystal length depends on the beam offset. According to the above considerations, we let the vertical beam offset 1 mm. That is equivalent to the pitch deviation of $8.06 \mu$rad. The detuning of the Bragg results in a flux drop of 67% at 25 keV.

The 1 mm small offset necessitates a well controlled overlap between the two crystals so that the input/diffraction beam will not be blocked. By the analysis of the geometrical relations among the two crystals, the input beam and the diffraction beam, we can find the adequate overlap is limited by 1.7 mm in the range of 7 keV–25 keV.

3.3. Adjustment mechanisms

Reduction of the adjustment mechanisms is another feasible strategy to increase the stability of the focus. The ray tracing[9] has been performed to find the tolerance of the six degrees of freedom for the beam stability. The yaw can be omitted because of its high tolerance(±5°). A sufficient crystal width can avoid the X translation. Similarly, the Y translation also can be omitted when the channel-cut concept(a long crystal) is adopted. The most important three degrees of freedom are the pitch, the roll and the Z-translation. The results of the simulation are shown in Table 2. If the demand of the positional deviation of the focus is 10 nm, the tolerances are $30 \mu$rad, 500 nard and 2 µm for the pitch($\Delta \theta$), the roll($\chi$) and the Z-translation(along the surface normal) respectively. Except the pitch(Bragg angle), the roll and the Z-translation, the second crystal must have a pitch fine tune for the mechanically tuning of the diffraction angle(See 3.2). In summary, the essential adjustments are a main rotation for adjusting the Bragg angle, a Z-translations on the first crystal, a roll and a pitch fine tune on the second crystal.

4. Expected performance and conclusions

The design concept of the small-offset virtual channel-cut monochromator is illustrated in this report. The stability of the sub-micron focusing will be benefited from minimization of the
thermal deformation and the reduction of the adjustments. Our analysis show that the total heatload can be reduced by confining the illuminated area of the crystal in a useful region and the power density dramatically drops when the monochromator is moved far from the source. Under such a condition, the thermal deformation can be minimize by a simple watering-cooling. For the reduction of the adjustment mechanism, our considerations are also shown in this report. The stringent requirements of the adjustments’ tolerances have been figured out by the optical simulation. Based on the above design, we expect the polychromatic flux is $1 \times 10^{11}$ photons/sec at least and the monochromatic flux is about $1 \times 10^{10}$ photons/sec at 15 keV The energy resolving power is better than 5000. The expected spot size is slightly small than 100 nm including the contributions of the slope error and the diffraction effect. The positional stability of the focus can be kept in around 10 nm.

**Figure 2.** Energy resolution, polychromatic and monochromatic flux at the sample position. The pink line with '□' represents for the energy resolution. The black line with '×' is for the monochromatic flux. The red line is for the polychromatic flux when the center of the selecting aperture is 1 mm high. The blue line is for the polychromatic flux when the center of the selecting aperture is 2 mm high.

| Spot Size (nm²) | $I_0$ (photons/s) | $\Delta v$ (nm) | $\Delta h$ (nm) |
|-----------------|-------------------|-----------------|-----------------|
| ideal | $53 \times 62$ | 1.0 | 0 | 0 |
| $\Delta \theta$ (μrad) | $53 \times 65$ | 1.0 | +30 | 0 |
| $\Delta \chi$ (μrad) | $53 \times 63$ | 1.0 | 0 | −31 |
| $\Delta Z$ (μm) | $53 \times 64$ | 1.0 | 0 | +12 |
| (μm) | $53 \times 67$ | 0.96 | +47.6 | 0 |

**Table 2.** Ray-tracing results for the three degrees of freedom. $\Delta h$ and $\Delta v$ are the position deviations of the focal point. $\Delta \theta$ is the pitch, $\Delta \chi$ is the roll and $\Delta Z$ is along the surface normal of the crystal. The spot size shown here is only the contribution predicted by geometry optics.

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