Design of New Protein Crystallography Beamlines

We have designed two high performance side-branch, asymmetric-cut curved crystal monochromator (ACCM) beamlines to fully utilize the sideway output of a superconducting multipole wiggler source for protein crystallography research. The optical layout of these two beamlines and the double crystal monochromator (DCM) beamline is shown in Fig. 1. The 13 mrad radiation fan of the wiggler output is shared by the three beamlines with optimization of the optical arrangements. Each of the two ACCM beamlines collects 1 mrad of radiation in the horizontal direction. One of them is located at 4 mrad and the other at 3 mrad away from the centerline of the radiation fan of the wiggler output. The central 2 mrad of the 13 mrad radiation fan is used by the BL13B double crystal monochromator beamline. Both of the side-branch beamlines reported here will deliver photon flux, through a 100 μm pinhole, of greater than 10^{11} photons/s with energies from 12 to 14 keV for standard monochromatic crystallography experiments. A Rh-coated, water-cooled vertical focusing mirror is placed upstream of the ACCM to simplify the energy tuning mechanism and to reduce the heat load of the crystal by cutting off the photon beams at energies above 15 keV. A novel monochromator that incorporates efficient cooling and precise bending mechanisms is designed and built in-house, as will be described in the following paragraphs.

A curved crystal monochromator is often used in hard x-ray beamlines because of its good energy resolution characteristics and focusing properties, especially for a side-branch beamline where space is a constraint. This type of beamline usually comprises one curved single crystal (Si or Ge), serving as both a monochromator and a horizontal focusing mirror, and one vertical focusing mirror. The photon beam is deflected sideways by the crystal at the Bragg angle and therefore a branch beamline can be added within a tight space around the central beamline. However, it is difficult to use this type of beamline for applications requiring continuous scanning of energy. The BL13A and BL-13C side-branch beamlines described in this report utilize such a design for crystal screening and other fixed-energy experiments, while the central beamline BL13B employs a double-crystal monochromator for multi-wavelength anomalous diffraction (MAD) and single-wavelength anomalous diffraction (SAD) experiments in protein crystallography studies.

The branch beamline with an insertion device source receives the output of the extended source laterally from an angle, and therefore sees a much larger source size in the horizontal direction than the central beamline. To reduce the effective horizontal source size, the branch beamline generally is positioned as closely as possible to the central beamline. Due to the constraints of space between the adjacent beamlines, the centerlines of beamlines BL13A and BL13C are located at 3 mrad and 4 mrad away from the centerline of BL13B, respectively. Both side-branch beamlines collect 1 mrad of the radiation, while the BL13B beamline collects the central 2 mrad radiation. The branch lines are designed to deliver photon beams in the energy range from 12 keV to 14 keV, by tuning the Bragg angle and optimizing the radius of curvature of the crystal.

The side-branch beamlines shown in Fig. 1 consists of a vertical focusing mirror followed by a curved crystal monochromator. The vertical focusing mirror in principle could be positioned before or after the crystal monochromator, as determined by various design parameters. The design considerations that lead us to position the mirror upstream of the crystal are as follows. First, the choice of reflecting material of the mirror affects the overall beamline design. Multilayer mirror coated with alternating layers of high-Z and low-Z elements is often used in x-ray beamline to increase the collection of photon flux, because the grazing incident angle of multilayer's reflection peak is usually greater than the total reflection angle of a coated mirror. By choosing appropriate layer thickness and materials, the multilayer behaves like a diffracting crystal but with a larger energy bandpass. Normally for a multilayer with constant layer thickness, the energy bandwidth is on the order of 10^{-2} to 10^{-1}. However, such a bandwidth centered at 13 keV is not large enough for the type of experiments that will be performed on the end-station, for which an energy tuning range about 2 keV is needed to cover the Se and Br absorption edges from 12 keV to 14 keV. Therefore, we choose a Rh-coated, Si-substrate mirror instead of a multilayer mirror.

The Rh-coated mirror is placed upstream of the crystal monochromator with a glancing angle of 4.5 mrad and a demagnification ratio of 4 to provide optimum vertical focusing at the sample position. Although the Rh-coated mirror is larger in the tangential direction than the corresponding multilayer mirror, it is still reasonably sized at 1 m for collecting the same amount of photon flux. Since the crystal monochromator has a tuning range of 2 keV, placing the Rh-coated mirror upstream of the crystal monochromator simplifies the energy tuning mechanism, which can be accomplished by simply rotating the crystal and end-station around the same axis. The additional benefit of an upstream Rh-coated mirror is the reduction of heat load on the crystal by attenuation of energies above 15 keV at the present glancing angle. As the first optical element after the Be window, the Rh-coated mirror received an estimated heat load of 35 W which is carried away by water-cooling Cu blocks attached to the sides of mirror.

Following the Rh-coated mirror, the photon beam is deflected sideways by the Si(111) asymmetric-cut curved crystal monochomator and passes underneath the photon beam of central beamline to the sample position. The curved crystal also serves as the horizontal focusing element and in this way, the number of optical elements is reduced. The asymmetric-cut crystal is employed to maintain the Bragg angle and good focusing property and to optimize the overall performance. Since the source size of wiggler seen by the side branch is larger than that by the central beamline, a high focusing ratio ~6 is used to effectively bring down the horizontal image size. As noted previously, this monochromator is designed for energy tuning from 12 keV to 14 keV. To satisfy optimum focusing condition in this energy range, the radius of curvature of the crystal is continuously adjustable from 60 m to 80 m using a bending mechanism shown in Fig. 2. The crystal and the bender mechanism are mounted on a goniometer assembly that allows proper alignment of the crystal and tuning of the diffraction angles for energies from 12 keV to 14 keV. At each diffraction angle the crystal is adjusted to the optimum curvature that provides the best focusing at the sample position.

As the second optical element the crystal has about 100 W of heat load deposited on its surface, and therefore adequate cooling is necessary to minimize crystal distortion and maintain optimum focusing condition. The design challenge is to integrate the cooling and bending mechanisms in one compact unit while maintaining their effectiveness. Existing designs for ACCM include internal-cooled thin crystal plate that is fragile and expensive to manufacture, or indirect/direct cooling that covers only partial surface of the crystal. To provide a cost-effective solution which has suf-

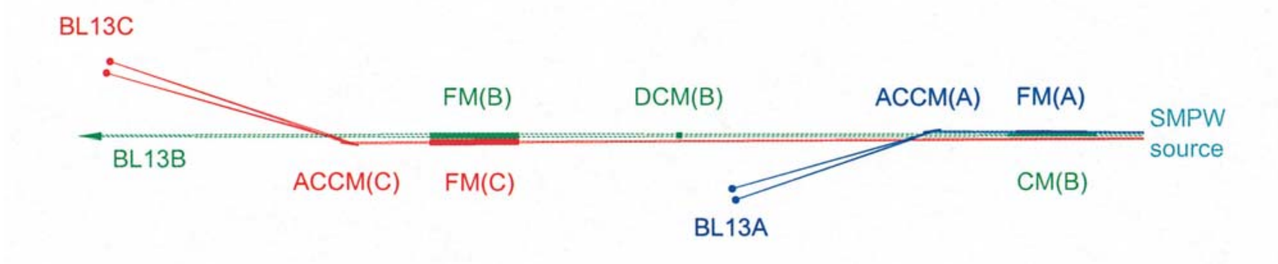

Fig. 1: Top view of the optical layout of the central and side-branch beamlines, which share the output of the Superconducting Multipole Wiggler (SMPW) source. ACCM: Asymmetric-cut Curved Crystal Monochromator. DCM: Double Crystal Monochromator. CM: Collimating Mirror, FM: Focusing Mirror.

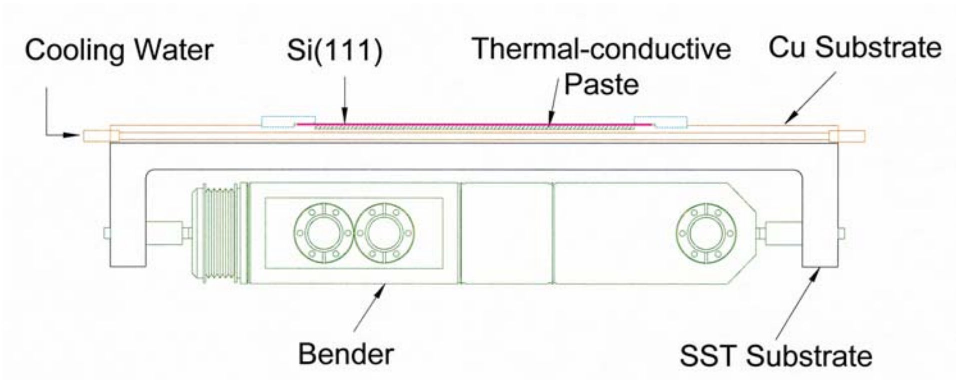

Fig. 2: Schematic drawing of the bending and cooling mechanisms of ACCM.

ficient cooling capacity and a reliable bending mechanism, we have designed a crystal monochromator that consists of a water-cooled Cu substrate brazed to stainless steel bender assembly, as shown in Fig. 2. The crystal plate is placed on the top of a recess on the Cu substrate and is clamped at both ends to the Cu substrate. There is no direct contact between the crystal plate and the Cu substrate except where the crystal plate is clamped, and it remains so during bending. The space between the crystal plate and Cu substrate established by the recess is filled by thermally conductive paste made from a proprietary mixture of Ga, In, and other metal powders. This alloy remains in the paste form from room temperature to above 100℃, and therefore adheres to the crystal and Cu surfaces without migrating or dribbling. It also adapts itself to the deformation of crystal plate and Cu substrate during bending. High cooling efficiency is achieved by an almost full coverage of the crystal plate by the heat-conductive paste. This design ensures that the monochromator will provide high photon flux and resolution while maintaining excellent stability.

In summary, we have designed a side-branch x-ray beamline with an innovate curved crystal monochomator that provides an energy tuning range from 12 keV to 14 keV. The layout is carefully designed to overcome geometrical constraints in the available floor space, and the optical components are chosen to meet the requirements of experiments. The crystal monochomator incorporates a new cooling and bending mechanism that should outperform current designs in terms of efficiency and stability.

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