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Beamline 14: a new multipole wiggler beamline for protein crystallography on the SRS

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A new multipole wiggler device has been designed for the 2.0 GeV Synchrotron Radiation Source at Daresbury Laboratory in the UK. The nine-pole 2.0 T device will provide radiation for two beamlines dedicated to protein crystallography, one of which will be of high intensity. This article provides details of the design of the two stations and outlines methods being developed to combine dealing with the high heat load from the radiation while allowing both stations to be built as close to the centre of the fan as possible.

Keywords: protein crystallography; multipole wigglers; beamline design.

1. Introduction

The Synchrotron Radiation Source (SRS) at Daresbury Laboratory in the UK is a well established 2.0 GeV second-generation synchrotron source providing radiation for a wide variety of experiments. In this article we present the outline designs for a new multipole wiggler (MPW) beamline on the SRS. The requirement for the beamline is to produce two stations dedicated to protein crystallography, one of which will be of high intensity. These two stations will complement the existing protein crystallography facilities at the SRS (Brammer *et al.*, 1988; Helliwell *et al.*, 1982, 1986).

2. Choice of insertion device

The desired range of wavelengths produced by the MPW is 0.9–1.7 Å. This requirement for accessing wavelengths in the 1.0 Å region necessitates a high-field magnet. The dipoles on the SRS have a 1.2 T field and a corresponding critical wavelength of 3.9 Å. To achieve the highest fluxes in the wavelength range required, a field of greater than 1.2 T is required. The practical upper limit on the magnetic field of a permanent-magnet MPW is approximately 2.0 T (Clarke, 1997). The maximum length of the insertion device is governed by the available straight section and is just over 1.0 m.

Calculations have been carried out to determine the optimum field, number of poles and gap of the insertion device. The minimum aperture possible in a straight section on the SRS before appreciable deterioration in beam lifetime occurs is 15 mm (Clarke, 1997). Therefore, after allowing space for the vacuum chamber, a reasonable gap to consider is 20 mm.

The combination of all of these factors has resulted in the specification of a 2.0 T nine-pole wiggler with a gap of 20 mm. A 1.8 T 11-pole wiggler would have produced slightly higher flux in the central portion of the fan at 1.2 Å. However, it would also have had a much more rapid fall-off in flux away from the centre of the radiation fan making the accommodation of a second high-quality station more problematic.

Fig. 1 shows a plot comparing the flux between the 1.2 T dipole, 6.0 T superconducting wavelength shifter and the 2.0 T MPW on the SRS. The power load at 1.2 Å is 182 W mrad^{-1} for the 2.0 T MPW, compared with 61 W mrad^{-1} for the 6.0 T wavelength shifter (at 300 mA). This indicates that the power loading from the MPW is high though it is less than that produced by multipole wigglers on other higher-energy sources (van Silfhout & Hermes, 1995; Padmore *et al.*, 1994).

3. Position of the stations on the fan

The MPW will deliver high-flux radiation to two stations dedicated to protein crystallography. With respect to total flux the optimum position for the two stations would be to place them symmetrically about the centre of the radiation fan. However, this has the significant disadvantage that neither station would receive the full effect of the on-axis X-rays from the MPW. In addition, as the horizontal acceptance angle moves off-centre the apparent source size becomes elongated, which reduces both the quality and quantity of the beam. Therefore, it is important to have both stations as close together as possible.

It is planned that each station will accept 4 mrad of radiation horizontally. The computer program *mpwangle* (van Dorssen *et al.*, 1993) has been used to determine the optimum location of the two stations on the horizontal fan of the beam. It is intended that the two stations will be separated horizontally by 0.5–1.0 mrad. This will allow space for the slits and mounting assemblies for the optical components. The total flux at three separate wavelengths (0.9, 1.2 and 1.5 Å) was calculated for various combinations of horizontal position and the most suitable one chosen.

The result is that station 14.2 will accept radiation from +3 mrad to −1 mrad and station 14.1 from −1.5 mrad to −5.5 mrad. In the event that a 0.5 mrad gap between the two beamlines provides insufficient physical separation between the lines then station 14.1 will accept −2 mrad to −5.5 mrad. The slight loss in intensity for station 14.2 which occurs by offsetting it by 1 mrad from the centre is more than compensated for by the gain obtained by moving station 14.1 nearer to the centre of the fan.

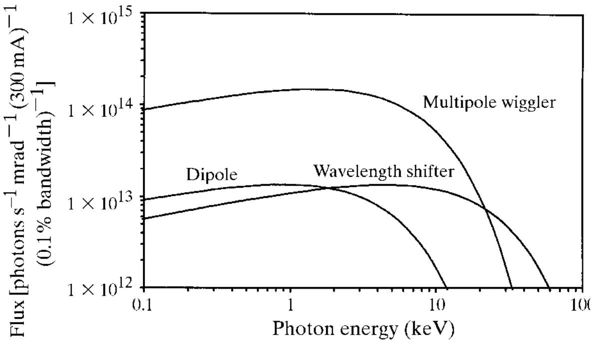

Figure 1
Comparison of the flux from a 1.2 T dipole, 6.0 T wavelength shifter and 2.0 T multipole wiggler on the SRS.

4. Optics

4.1. *Optical elements*

A major requirement for protein crystallography at the SRS is for facilities to carry out high-resolution data collection on weakly diffracting crystals. As a consequence, the optics are being designed for fixed-wavelength operation rather than rapidly tunable operation. A cylindrical mirror will provide the vertical focusing and a cylindrically bent triangle monochromator will both monochromate and horizontally focus the beam. The optical elements for both stations have been designed to ensure that the stations operate at two wavelengths: station 14.1 at 1.2 and 1.5 Å and station 14.2 at 0.9 and 1.2 Å. The higher wavelengths were chosen due to the increased flux: a factor of 1.5 times more flux (at the centre of the fan) exists for 1.5 Å than 1.2 Å. In addition, the scattering power of the sample is greater at higher wavelengths so a combination of these two effects would result in lower exposure times being required. The longer wavelengths would be suitable for small frozen crystals where absorption errors are low. The intention that station 14.2 be able to access wavelengths around 0.9 Å is to allow work at the selenium *K*-edge at 0.979 Å. The demand for the ability to carry out experiments at the Se *K*-edge is rapidly increasing as the biochemical techniques required for producing proteins containing selenium-labelled methionine residues are becoming more routinely employed. It is certainly feasible that the method of using the signal from the selenium engineered into the protein will become the preferred method of solving the phase problem in the near future. It is not intended that the new facilities replace the existing experimental stations operating in the 1.0 Å region; rather that they complement them, providing a higher-flux alternative. In practice, each station will be characterized at two wavelengths during commissioning and then demand will determine the choice of wavelength for routine operation.

Given that this beamline is being built on a well established storage ring, there is very little room for flexibility regarding the positioning of the various optical elements on the beamline. The shield wall occurs at 14.5 m from the tangent point, so in order to allow routine access, all optical elements must be placed beyond this point. In addition, the beamline must also cross the transfer path between the booster and the storage ring itself.

Both stations will be equipped with 1.2 m mirrors manufactured from silicon and coated with rhodium and inclined at 3.5 mrad. The overall geometry of the beamline means that the first possible position for a mirror (for station 14.2) is at 16 m from the tangent point. The mirror for station 14.1 is at 20.5 m. The choice of mirror length and inclination was made on vertical acceptance combined with producing a focus where optical aberrations do not dominate.

Monochromation of the beam will be provided by bent triangle monochromators. As has been stated earlier, it is planned that the horizontal aperture of the two stations will be separated by 0.5–1.0 mrad. The bending and cooling mechanisms for the monochromators will be mounted on the back face of each crystal. The reflected monochromatic beam for station 14.2 will pass across the white beam for station 14.1 so that the mechanism for the 14.2 monochromator does not shadow the 14.1 beam. Fig. 2 shows a schematic layout of the beamline indicating crossing of the individual beams to form stations 14.2 and 14.1.

Monochromation for station 14.1 will be provided by two Ge(111) monochromators mounted together in a vertical stacking arrangement. The two monochromators will be optimized for work at 1.2 and 1.5 Å. Station 14.2 will have an Si(111) monochromator for work at 0.9 Å and a Ge(111) monochromator for work at 1.2 Å, again mounted in a vertical stacking arrangement. The asymmetry of the cut of the monochromators will allow a source demagnification in the region of 10:1.

4.2. *Heat loading*

The front end of the beamline is designed to have a transmission of greater than 80% at 1.2 Å. As this wavelength is much less than the critical wavelength of the magnet (2.3 Å), much of the power can be absorbed in the front end rather than on the optical components. The mirrors will be inclined at 3.5 mrad and thus will reflect all wavelengths above 0.65 Å. The estimated power absorbed by the mirrors will be in the region of 4 W mrad^{-1}, which is unlikely to cause any significant damage or distortion to the optical surface of the mirrors. However, it has been decided to cool the mirrors to avoid any problems which might occur as the mirrors and their mounts thermally cycle during any machine fill.

After absorption in the front end and reflection off the mirror, the power incident on the monochromators is approximately 80 W mrad^{-1}, over 300 W in total. This will produce significant distortion of the monochromator surfaces unless some form of cooling is implemented. A cooling scheme is being devised to produce a slope error of less that 5 arcsec along the cylindrically bent monochromator. This slope error will produce approximately a 10% increase in horizontal focal spot size.

4.3. *Experimental set-up*

Both stations will be equipped with a 2θ arm coupled to the angle of the monochromator in order to accommodate the change in beam position with wavelength. The precise make-up of the station goniometry and detectors has yet to be determined. However, it is certain that the final choice will allow high-resolution protein crystallographic data to be collected quickly and easily.

5. Conclusions

The SRS is the oldest second-generation synchrotron X-ray source in existence. Although its source size and modest energy means that it cannot provide X-ray beams with the high brightness or flux obtainable on some of the more modern third-generation X-ray sources, we have demonstrated with the design of this beamline that a high-intensity protein crystallography facility on the SRS is feasible. The projected performance of the beamline compares very favourably with that of the popular existing beamlines on the SRS. The beamline has

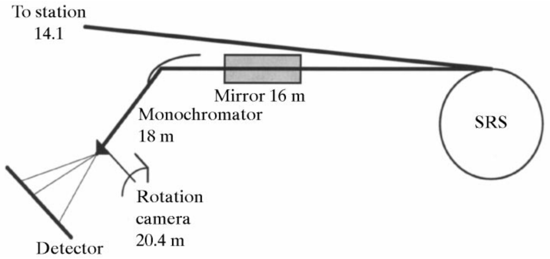

Figure 2
A schematic layout of beamline 14.

also been designed so that it would be transferable to a multipole wiggler or bending magnet on the proposed third-generation X-ray source, DIAMOND, planned to replace the SRS at Daresbury in the near future.

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