Optical designs and tolerances for the 8.3.1 protein crystallography beam line

M. R. Howells, 9-3-99

Introduction

This beam line arose out of discussions between Howard and the user group at UCB (Alber, Berger et al). It was based on the novel concept that protein cyrstallography beam lines do not need a high-power insertion device such as an undulator on a high energy machine or a wiggler on a medium energy machine (like the ALS). In fact, if the sources and optics of such beam lines are designed to be as efficient as we know how to make them, then the protein crystal reaches a damage threshold, which is about 10^{10} incident photons per square micron, in seconds or less. As a consequence, the normal process of crystallography, consisting of interleaved periods of data collection and detector readout, becomes very difficult to arrange. Moreover, since most of the time is spent reading the detector, the rapid rate of data recording contributes little to improving the overall speed of the process. The result is that people often intentionally reduce the intensity of the beam with absorbers. Furthermore, the inconvenience of excessively high power x-ray beams is not limited to the experimenter. It also leads to much more difficult and expensive engineering solutions for the basic beam-line systems such as mirrors, monochromator crystals, beam-defining apertures, radiation shielding and so forth.

Given the understanding now developed by Howard of the true source requirements for crystallography, we know that the important property is the horizontal source brightness (measured in ph/sec/mr/mm/0.1%BW). Thus if we have a source of sufficient brightness but *low power compared to an insertion device*, then we should be able build a much simpler and less expensive beam line that is nonetheless capable of reaching the protein-crystal damage threshold in a time of the order of a minute. (in the case of an ALS beam line of the type discussed here, the actual numbers at 12 keV are about 50 seconds for a superbend and 250 for a normal bend.) This is still fast enough that the experiment time will continue to be dominated by the readout time of the detector for some time to come. An ALS superbend therefore offers the opportunity to build beam lines for protein crystallography and other applications with relatively low power components and without incurring the cost of an insertion device or the need to commit a scarce straight section. So that is the goal of the present and several upcoming projects at the ALS.

Optical design: general layout

The original optical design is shown in Fig. 1. It was developed by Howard before I became involved in the project. It is also virtually the same as the adopted design but the final decision in favor of that scheme took some time and study. The principal design parameters now are:

Table 1: Basic dimensions

Quantity	**Unit**	**Value**
Vertical source (FWHM)	μm	20 (8.5 rms)
Horizontal source size (FWHM)	μm	220 (94 rms)
Vertical collection angle	mr	0.5
Horizontal collection angle	mr	3
First mirror distance	m	6.5
Second mirror-to-sample distance	m	3.25
Source-to-mono distance	m	16
Mono-to-sample distance	m	16
Horizontal magnification		1
Vertical magnification		0.5

- First Howard had considered several alternatives including a scheme involving toroidal mirrors (Fig. 2). He wanted to have a sound basis for eliminating these. The toroid scheme had inferior (but still marginally acceptable) imaging performance compared to the first design and allowed use of a flat crystal monochromator i. e. without the sagittal-focusing crystal.
- I made an investigation of similar beam lines at other places and constructed the chart of Fig. 3.
- I had already made a calculation using standard plate theory to assess the errors of bending the beam line 4 refocusing mirror. This is the one built by Dawn Munson which was shaped so that one would expect plate, rather than beam, behavior. Therefore I could easily study the sagittal-bending crystal problem using my existing code. Results were that the well-known “anticlastic bending” effect could be controlled by making the crystal large enough without the use of ribs which are hard to make and even harder make with good back and front accuracy of the plate to be bent. The quantitative result was that a crystal 100x130 mm stiffened down the two straight edges would hold its cylindrical shape within sufficient accuracy (see later) over the illuminated area (at 12 keV) which I took to be 48 mm sagittally and 16 mm tangentially. This encouraged us to think that we

could build the sagittal crystal reasonably easily which would not have been the case if it had needed ribs.

- The problem with the two-toroid scheme is that we have no long-term reliable source of high quality cooled toroids, i. e. cooled and bent cylinders. This essentially requires an internally-cooled metal mirror, since, at least according to me, side cooling is a sound strategy only if one does not at the same time have to do bending. Such cylinder vendors as there are mostly offer ceramic mirrors which cannot easily be used in internal-cooling designs.
- The balance of issues is shown in the chart of Fig. 4. Added to that we have lots of expertise in bending here in ALS while for procuring difficult mirrors we would have to place reliance on some rather flaky small-business people. The conclusion was to go with the sagittal-focusing optical scheme.

Optical design: choice of parameters

The tradition in x-ray crystallography is to deliver the light to the sample (the protein crystal) via a 100μm diameter pinhole known (somewhat inappropriately in my view) as a collimator. Although at time of writing the design of the hardware around the sample has not yet been resolved, we assume for this discussion that the collimator will be there. Its size is determined by the size of the crystals that people grow of interesting macromolecules. Thus we have two simple ways to arrive at optical tolerances. One is to require that the brightness of the source be preserved. The other is to require that the beam be delivered into the 100 μm collimator with divergence below about 3 mr. The divergence requirement comes from the need to have neighboring diffracted orders sufficiently separated and in fact the angles at the delivery point are 3 mr (H) and 1 mr (V). These values follow from the collection angles at the source and the horizontal and vertical magnifications given in Table 1.

Consider first the horizontal size. The geometrical image width (derived from the table) is 220 μm so we lose about a factor two in flux due to overfilling of the collimator. This is the situation where the horizontal source brightness determines the deliverable flux. If we reduced the horizontal magnification to 0.5, the spot size would go down to 110 μm and the convergence angle would go up to 6 mr. Thus we gain a factor two in matching the spot size to the collimator but lose it again because we must reduce the convergence angle back to 3 mr by some form of aperturing. Only a greater number of ph/sec/mr/mm/0.1%BW would allow an improvement. This is not bad news since the ALS has a very good value of the horizontal brightness compared to other sources. An interesting sidelight is that a beam line with a horizontal magnification of 0.5 is no worse off than ours for flux and is a better choice

from a floor layout point of view as the closest neighbor to a unity-magnifying superbend beam line. The general requirement is that at least two different values of the magnification are needed for a superbend pair in order that the experiments come out at different distances from the source and thus have enough space. As we will see the horizontal optical tolerances are less difficult than the vertical ones on account of the forgiveness factor at the crystals as well as the larger source size and the fact that the mirrors do not contribute any important limitations because they have enormous forgiveness factors. Thus we expect that the horizontal spot size will be achieved without difficulty and without degradation of the horizontal brightness.

We now turn to the vertical spot size which is much more problematic. The vertical FWHM spot size at the sample delivered by a perfect optical system would be 10 μm (from Table 1). This would preserve the source brightness but requires the tolerances shown in Table 2 which are very difficult. Moreover, crystals as small as 10 μm, although they exist, are extremely hard to work with because the radiation damage is shared among a much smaller number of macromolecules. As a consequence they provide much less data (maybe only one cycle) before they die and hundreds of crystal changes may be needed to collect a full data set. Consequently people always use larger crystals if they can and as a result a 100 μm FWHM spot is a much more common requirement. Moreover, if we had a 10 μm focal spot we would spend most of the time deliberately spoiling the focus so as to fill the 100 μm collimator. Further if we have a 100 μm spot we can always reduce it to 10 μm by slits. This is not as good as a sharp focus because it loses flux but at our projected x-ray intensity of $2x10^8$ ph/μm^2/sec in a 100x220 μm spot, it is still quite good.

Based on these facts and discussions with our user community we have decided to adopt as the standard beam line performance, a delivered spot size of 100x220 μm with a goal of 50x220.

Calculation of optical tolerances

The standard way to calculate optical tolerances based on a Gaussian source of rms width Σ is as follows. For a source at distance *r*, the allowed rms slope errors (σ) on the first mirror are

Tangential plane: $\sigma_t \le \Sigma_t/(4r)$,

Sagittal plane: $\sigma_s \le \Sigma_s/(4r\sin\theta_G)$,

where θ_G is the grazing angle. The argument is that the mirror forms a virtual image of the source which must not be degraded in rms size by more than about 10%. If the errors are Gaussian then the resultant rms image width is the quadratic sum of the rms width of the blurred virtual image of each point of the source with the original rms source size. If the rms blur width were equal to $\Sigma/2$ then we would have a resultant width of $\Sigma\sqrt{1^2 + (1/2)^2} = 1.118$ which is just about tolerable. Including another factor two because the optical ray is deviated by twice the mirror surface slope error, we arrive at the factor 4 in the above equations. The FWHM source sizes (*S*) are 2.35 times larger than the rms ones ($S_{\mathrm{FWHM}} = 2.35\sigma$).

If achieved, these tolerances are intended to guarantee preservation of source brightness. They are calculated here for the first mirror but similar arguments apply to the errors on any of the optical surfaces. For example the first mirror in this system is a collimator in the vertical so tangential errors on any other optical surface would produce the same degradation of the source size as if the error occurred on the first mirror. Imagine the rays reversed to see this.

To convert to the angular tolerances needed to deliver a final spot of rms size 43 μm (FWHM of 100μm) we set Σ_s or Σ_t equal to 43 μm and *r* equal to the focal distance of the final mirror. These results of these calculations are shown in the following spread sheet.

Optical tolerances

Basic dimensions	Unit	Value	RMS values
Vertical source size (FWHM)	µm	20.00	8.51
Horizontal source size (FWHM)	µm	220.00	93.62
Vertical collection angle	mr	0.50	
Horizontal collection angle	mr	3.00	
First mirror distance	m	6.50	
Second mirror-to-sample distance	m	3.25	
Source-to-mono distance	m	16.00	
Mono-to-sample distance	m	16.00	
Horizontal magnification		1.00	
Vertical magnification		0.50	
Bragg angle min	deg	7.00	
Bragg angle max	deg	20.00	
Bragg angle 12.5 keV	deg	9.00	
Mirror grazing angle	deg	0.26	
Collimator size (full width)	µm	100.00	42.55

Slope errors	Brightness preserving (µr)	Collimator driven (µr)
M1 rms slope error: tan	0.33	3.27
M1 rms slope error: sag	800.15	727.41
Crystal rms slope error: tan	0.33	3.27
Crystal rms slope error: sag	23.02	20.92
		(at 12.5 keV)
M2 rms slope error: tan	0.33	3.27
M2 rms slope error: sag	800.15	727.41

Each calculated as if it was the only error

Optical design tolerances for the whole beam line

Obviously we have four optics to consider and the overall errors will be roughly a quadratic sum of the individual ones. It is clear from the spread sheet that we have nothing to worry about in the sagittal plane as argued earlier. The hard part is holding tolerances in the tangential plane. This means that we have to plan an error budget that can deliver an overall error of 3.27 µr rms. We expect the dominant errors to be as follows.

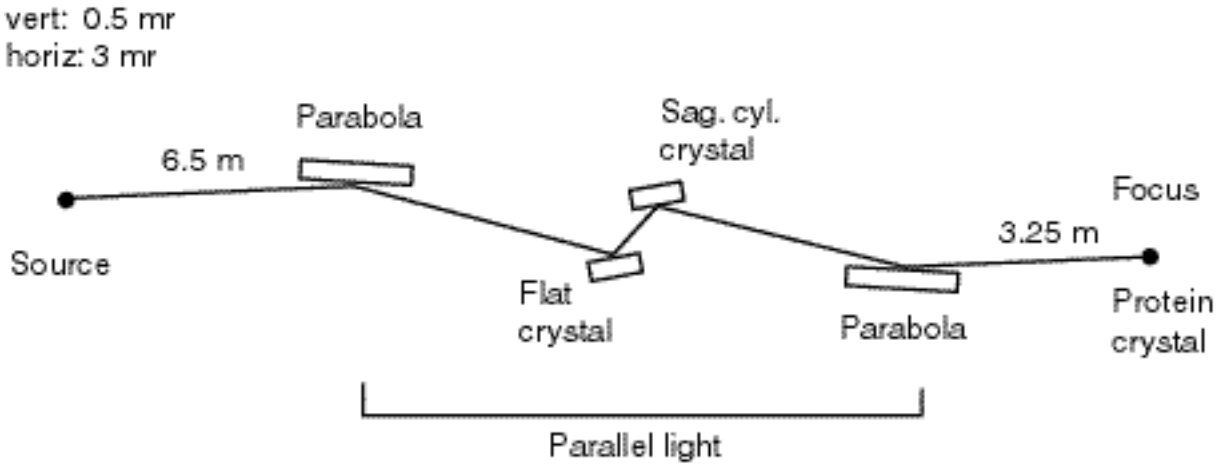
M1 mirror	Optical fabrication errors, thermal errors are negligible
First crystal	Thermal errors, Bragg planes are atomically flat
Second crystal	Bending strains producing non-flat Bragg planes, thermal load is

	negligible
M2 mirror	Optical fabrication errors, thermal load is negligible

Roughly speaking if we aim for 2 μr in each surface we will get $\sqrt{2^2+2^2+2^2+2^2} = 4$ μr rms overall. To get 3.27 μr overall we would thus need 1.64 μr at each optic. Instead we are aiming for 2 μr. This is not an exact science!

Crystal designs and monochromator issues

At the time of this writing the thermal studies of the first crystal and bending experiments on the second crystal are still unfinished. Therefore in order to get this report out in reasonable time we defer those questions to a later report.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Parabola
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Parabola
Protein
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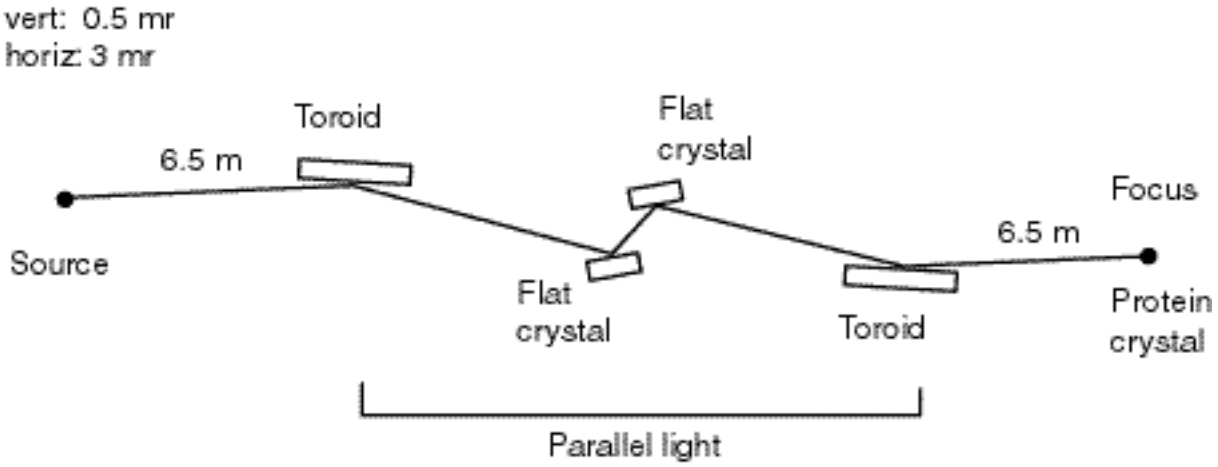
Parallel light

Fig. 1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Toroid
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Fig. 2