

UPBL9b: Pump-probe and time-resolved experiments

Current designated sector:	Facility goes to:
ID09b	ID09

1.1 SUMMARY

We propose a dedicated beamline UPBL9b for time-resolved diffraction and scattering in physical, chemical and biological systems. The time resolution will typically be obtained in a pump-probe fashion where the samples are initiated by short laser pulses. The experiments will be conducted in the following way: short laser pulses initiate a reaction in the sample and the diffraction (or scattering) from delayed X-ray pulses probe the structure in that delay. A film of the atomic motions is obtained by stitching these snapshots together for many time delays. For slower millisecond processes, a time resolved area detector will record the full time-history in one sweep hereby greatly enhancing the efficiency of the experiment. The time resolved area detector should open up new experimental opportunities for handling irreversible experiments and experiments that cannot be initiated by light.

An inherent challenge in laser initiated SAXS & WAXS experiments is the thermal signal from the bulk which “lies on top” of the structural signal. To remove that signal, infrared laser pulses will be used to transiently heat the bulk sample without initiating the structural transition itself. Hence the intrinsic structural signal can then be obtained by subtracting of the two components after suitable normalisation. The quality of the structural data will greatly improve since the two measurements will be done on the same sample.

The extreme intensity of the X-ray beam on UPBL9b will make it possible to initiate certain reactions with the X-ray beam itself. For example if water is exposed to a very intense beam, the photo electrons will migrate, within nanoseconds, into crystal-like cavities with the electrons in the centre. The structure around this solvated electron has been predicted theoretically but the calculations have not been checked experimentally.

An optional X-ray emission spectrometer will be build around the sample for probing the spin- and oxidation-state dynamics of transition metals which will be very useful for metallo-enzymes that catalyse chemical reactions in living organisms.

The X-ray beam will most likely be produced by two short-period undulators U14 where the radiation is concentrated on the first harmonic. That lowers the heat load on the optics and the choppers which is a tremendous advantage. In return the energy tunability is limited. The first U14 harmonic can be varied from 18 to 24 keV, the third harmonic from 54 to 72 keV. Operated in tandem the undulators produce 1.2×10^{10} photons per pulse in a 5% BW at 18 keV, i.e. 7.5 times more than the flux available on ID09 today. And by reducing the focus from 100 to 50 μm with a high-demagnification toroidal mirror ($M=0.4$), the flux density will increase by a factor 30. Combined with a fast-read-out detector, the number of time delays (or number of samples) that can be measured in one day will increase dramatically. The high-energy $3E_f$ beam will triple the spatial resolution in some cases down to a sub-atomic level of 0.25 Å. At very high spatial resolution, the scattering from a liquid is independent of its structure, i.e. it depends only on its atomic content. Getting access to this high-Q limit, the scattering will be normalised to the atomic scattering which does not change during a structural change. The scaling of *laser-on* (excited state) and *laser-off* images becomes straightforward which will make the data more trustworthy.

1.2 PROJECT HISTORY

ID09 has currently two experimental hutches, a high pressure hutch for beamline ID09A, and a downstream hutch for time resolved experiments for ID09B. Beam time is shared 50%-50% between the two stations. ID09B is exclusively used pump-probe experiments which can now be done routinely with time resolution of 100 ps time limited by the 100 ps X-ray pulses at the ESRF. The demand for beam time on ID09B is oversubscribed by a factor 3-4 with proposals in physics, chemistry and biology. Over the last three years there has been a shift towards SAXS/WAXS due to the higher success rate of these experiments in spite of the lower information content. With this demand for beam time, the user community is stifled and we wish therefore to double the available beam time in UPBL9b. In practice that means accepting more proposals and giving more beam time to demanding experiments. In the first upgrade proposal, ID02 and ID09B were merged onto one beamline, UPBL9 but it was impossible to combine the high flux demand for TR experiments with the high collimation demands in USAXS/SAXS experiments (conflicting low-beta/high-beta site requirements). In the present proposal ID02 will be extended with a USAXS hutch and become UPBL9a. ID09B will stay on ID09 and change name to UPBL9b. ID09A will move to ID15.

The issue of synergy between UPBL9a and UPBL9b was discussed during the brainstorming in December 2008. Participants overwhelmingly supported the proposal which led to the conclusion that there is a strong potential for new science from this unique combination. For instance, many solution phase sub-millisecond and microsecond SAXS experiments will be flux limited on UPBL9a. This class of experiments could be moved to UPBL9b provided that a suitable SAXS chamber is built. That is more cost efficient than providing pink options on UPBL9a considering the complexity of handling hot beams (water cooling, shielding etc.). The complementarity of these SAXS options will give the beam-time-review-panel the flexibility to exchange life science proposals between the two instruments, depending upon their scientific merit and oversubscription factor. In addition, the high-energy SAXS option on UPBL9b is an advantage for sub-millisecond pressure-jump experiments. Sample environments such as laser temperature-

jumps, pressure-jumps, stop-flow and micro fluidic flow devices, detectors, and sample preparation lab will be shared between the two branches.

The UPBL9b project was presented at the SILS meeting in Palermo, June 28, 2008, at the Centre for Molecular Movies in Copenhagen, July 2, 2008 and at the Nordic Femtochemistry Conference in Århus, October 2-4, 2008. The project was always very well received. The detailed project was examined and discussed at the UPBL9 brainstorming in 15-16 December 2008.

1.3 SCIENTIFIC CASE

Introduction

The prime purpose of UPBL9b is to molecules in time by scattering or diffraction at the highest possible spatial and temporal resolution. Can we locate the active atoms in a molecule? Are there several pathways? How many intermediates are there and what are their time scales? What is the role of the environment? These questions are complicated and can only be answered if a large number of molecules are excited by the laser (better S/N ratio).

The first ultrafast film of a protein at work was recorded in 1994 on ID09B in a Laue study of CO dynamics in myoglobin. The following films on myoglobin mutants, haemoglobin and PYP have provided new insights into the structure function relationship in protein dynamics [1,2]. When the sample is non crystalline, the X-ray scattering is diffuse and the information is reduced to scattering curves $\delta S(q, t)$ that oscillate around zero. The new work form ID09B on haemoglobin has shown that the $\delta S(q, t)$ curves are very sensitive to changes in local and global structure [10]. Solution work thus is increasingly important since it allows studying many more systems under physiological conditions freed from the constraints in crystals.

Pump-probe experiments require time for experimentation and this was sometimes compromised in the past when too many experiments were scheduled in too few shifts. With a dedicated UPBL9b, the allocations could be increased from 9-12 shifts to 15-18 shifts and long-term proposals could be accepted without blocking access for other users.

At the highest time resolution, single X-ray pulses are isolated by a chopper from one of the four single-bunch filling modes of the storage ring. The chopper needs a time gap in the bunch structure of about 300 ns to isolate the pulse from that bunch. The current single pulse modes are 4-bunch mode, 16-bunch mode, hybrid mode ($24 \times 8 + 1$) and the $7/8+1$ mode. With the latter now being the default mode, the available beam time for single-pulse experiments has increased from 35% to 80% with the remaining 20% in uniform mode. The time resolution in uniform mode is given by the minimum open time of the chopper, 265 ns. That corrects a frequent misunderstanding that pump-probe experiments can't be done a uniform fill.

Static and time-resolved studies in the sub-millisecond range

As mentioned in the project history, UPBL9b is expected to take all life science related sub-millisecond experiments from UPBL9a. The periods in uniform fill are

ideal for that. This will enable, for example, recording of the changes in weak layer line reflections associated with rapid molecular events during active contraction and force recovery in single muscle fibre with sub-millisecond resolution. Other examples include microsecond conformational changes in proteins such as folding and diffusive reactions induced by pressure or temperature jumps. Ideally the whole time history could be filmed with a high-frame-rate pixel detector. A similar approach could be used to track the signal corresponding to rapid water redistribution during pressure-induced structural transformation in lipid membranes (e.g. lamellar to inverse bi-continuous cubic phase transition). Pink beam capability combined with rapid mixing techniques (stopped flow/quenched flow) will be beneficial for a variety of kinetic studies in the millisecond range induced by concentration or pH jumps involving very dilute systems. Finally, accurate static characterisation is a prerequisite for any time-resolved experiment. This type of pre-characterisation could be undertaken during the uniform filling mode.

Time resolved crystallography

The structural dynamics of small proteins like myoglobin and haemoglobin, the yellow protein (PYP), the green fluorescence protein (GFP), bacteriorhodopsin (bR) have been studied by time resolved Laue diffraction for 15 years on ID09B. It is now possible to measure the correlated structural changes around active sites to a time resolution of 100ps [1]. UPBL9b will tackle more complex and larger proteins that are more important biologically. Take the photosynthetic reaction centre (RC) for example, where the large unit-cell and small crystal size are on the limit of being possible today. Richard Neutze recently measured the motion of a key tyrosine in RC on ID09B which shows how the photo-induced electron transfer drives a large scale relaxation which is fundamental in photosynthesis. With smaller more intense beams, we will work with smaller crystals ($10\ \mu\text{m}$)³ and the signal-to-noise ratio should improve from using more sophisticated laser technology (see later). With recent advances in chopper technology, the intensity of the X-ray pulse can be optimised by adapting the pulse duration to the needed time resolution: nanosecond dynamics will be probed by 100 ps pulses, microsecond dynamics by 100 ns pulses etc. Likewise by adapting the laser pulse-length to the time evolution in the sample, the sample can be excited more efficiently and with less radiation damage. One component of the laser-radiation-damage is multi-photon absorption, which is proportional to powers of the intensity I^N . So for example if a pulse is stretched by a factor ten in time, the two-photon cross section in the long pulse is $(1/10)^2 = 1/100$ lower. Note that the signal-to-noise-ratio (S/N) of a weak photo-signal on a high background is proportional to dN/\sqrt{B} , where dN is the number of excited molecules and B the background. So by doubling the number of excited molecules, the S/N ratio is also doubled. A similar gain would require a four times longer exposure with the X-rays. That shows the importance of exciting the sample efficiently. The excitation level in the most known photo proteins is around 10-20% with the sort laser pulses used today (0.1ps). If we can increase the concentration of excited molecules, the higher S/N ratio should give us cleaner maps with more details.

Another important area is ultra-fast phase transitions in organic crystals. Eric Collet (Rennes) and colleagues are now designing materials where the electric and magnetic properties can be changed with a laser pulse [3]. This is important for optical switches, data storage and high-speed communication. This field will greatly

benefit from a smaller and more intense beam at higher energies. Sample positioning will be done with a 4-circle goniostat for a more complete sampling of k-space and the new laser technology will increase the S/N ratio. Solid-state transitions are traditionally triggered optically, but some transitions might be triggered more efficiently by single-cycle THz laser pulses that couple directly to the (THz) phonons in the sample. The THz pulse can be produced by optical rectification of an intense 800 nm femtosecond pulse in a LiNbO₃ crystal [4].

Recently the Centre for Molecular Movies in Copenhagen has initiated studies of the grazing incidence scattering from organic thin films. These materials and their confined geometries have great potential in organic electronics and photonics applications. The grazing incidence geometry offers the advantage of matching the penetration depth of the optical excitation with the volume probed by the X-rays, since varying the incidence angle allows controlling the penetration depth of the X-rays. The small incidence angles require a well collimated X-ray beam with high stability, better than 1 μm and 1 milli-degree. UPBL9b will provide time resolved grazing incidence SAXS, which is increasingly important for studying the shape of nanostructures in devices, e.g. at buried interfaces.

Time resolved protein structures in solution (SAXS/WAXS)

The first sub-ms SAXS/WAXS study of a protein in solution was done in 2005 on D09B [5]. The transition from ligated to non-ligated haemoglobin (HbCO) was measured with a pink beam (3%bw). The experiment showed how CO dissociation drives a large conformational change, the well-known Relaxed (R) to Tense (T) quaternary transition. In this transition the sub-units α_2 and β_2 rotate 25° in 2 μs . The solution structures of HbCO and Hb agree quite well with their crystal-counterparts after angular averaging. The results surprised everyone: the relative protein-to-water signal is much higher than for small molecules, typically 1% with a protein concentration of 1 mM (2.5% volume fraction). The protein is scattering as a gas of independent molecules with a forward scattering proportional to Z^2 , where Z is the sum of all the electrons in the protein (37516 electrons/Hb). In addition the scattering from water is weak in the SAXS/WAXS range 0.01-1 \AA^{-1} where the Hb signal $dS(q, t)$ is strongest due to the length scale involved. UPBL9b will provide a SAXS chamber with a pixel detector that will allow probing protein changes on length scales up to 500 \AA .

The haemoglobin work has sparked off a new demand for beam time in part to check if proteins in their natural environment behave as in crystals. Even more important are these photo proteins that cannot be crystallised. Protein folding is another area which might become important and the first applications for beam time are beginning to come. By triggering protein folding from a cold unfolded state with an infrared laser pulse, we might be able to monitor the folding process in real time.

SAXS/AXS experiments are currently done on ID09B with the asymmetric energy spectrum of the pink beam (3%bw) which tend to dampen $\delta S(q, t)$ as compared to monochromatic curves. Although the asymmetric spectrum can be included in the theoretical curves before the fitting, this has proven difficult to do precisely due to unknown angular and energy dependent terms in the detector. In reality the effective X-ray wavelength is only known to a precision of 2-3%. With the recently installed multilayer monochromators, the spectrum is made Gaussian and the

bandwidth can be varied from 0.1 to 3%. It is now possible to measure bond lengths and angles more precisely.

A photon counting pixel detector is ideal for SAXS/WAXS work due to the lower angular scattering compared to crystals which ensures that a pixel is not hit by more than one photon per pulse on average. The time resolution of the Pilatus detector is presently 50 ms but it will soon be improved by one order of magnitude. The prospect of filming the time-history in a string of images would dramatically improve the efficiency: one laser shot followed by hundreds of images. The pixel detector could initially be shared with UPBL9a.

Time resolved solute structures in solution (WAXS)

This field started with dissociation & recombination studies of small molecules such as I₂, Br₂, Hgl₂, HgBr₂, CH₂I₂ and C₂H₄I₂ [6-8]. The aim is to determine the structure of the photoproducts and their populations from 100 ps to 1 ms and over distances from 2-20 Å. The solvent is an active partner that might boost certain reactions. From the scattering curves $\delta S(q, t)$ it is possible to deduce the change in the internal and external structure of the molecules and the hydrodynamics of the solvent.

Solution experiments are confronted with a problem: the formation of new structures is usually accompanied by a change in the total energy of the molecule. That leads to exchange of energy with the solvent which typically cools the newly formed molecules. How is the solute signal extracted from the total signal? We have recently learned how to measure the scattering signal from the heated solvent alone by exciting non-destructively with infrared laser pulses. In this way the solvent molecules don't change internal structure but they transfer heat to the solvent within picoseconds as they relax back into thermal equilibrium. UPBL9b will provide infrared beams from a parametric amplifier (TOPAS) for this purpose.

As X-ray scattering probes *all* structural changes in the sample including solvent heating, it is a complementary tool to X-ray spectroscopy which is a local, element specific probe. It would be nice to have a XANES/EXAFS option on UPBL9b but that would require unique X-ray optics (high energy resolution, collimating mirror etc). It is probably easier to add an X-ray emission spectrometer as the one build by Pieter Glatzel on ID26 which can be used with a pink beam.

Small molecules will greatly benefit from higher X-ray energies that will increase q_{\max} from 8.5 up to 25.5 Å⁻¹ in ideal cases of strongly scattering samples. A simulation of the iodine transition: I₂ → 2I in CCl₄, predicts that we will resolve seven oscillations in $\delta S(q,t)$ above the noise floor (54 keV, 1 x 10¹³ photons, 25 s exposure, I₂^{*} concentration 1: 10⁴). To shorten the exposure time at higher energies, the pump-probe frequency could be increased from 1 to 3 kHz with a new high-speed chopper (see later).

The high energy beam will give access to the high-q part of the scattering function S(q) where molecules scatter as the sum of independent gas atoms. The atomic range starts > 15 Å⁻¹. In this high-q range, the scaling of laser *on* and laser *off* is straight forward which makes the difference scattering more reliable.

Finally, the Centre for Molecular Movies in Copenhagen is developing a micro fluidic sample cell with integrated optical characterisation. With the tighter focus on UPBL9b (40 μm), this design can be realised in a windowless configuration using capillary-burst-valves, whilst maintaining the high flow speeds which are needed for replacing the sample at kHz rates. The new jet will be particularly useful for difficult-to-obtain or -prepare samples.

Gas phase reactions and laser slicing

At the UPBL9 brainstorming Brian Mitchell (Rennes) and Hyotcherl Ihee (Kaist) mentioned that gas-phase photochemistry is important in quantum chemistry (check of the simplest DFT calculations, branching ratios etc.) and that X-ray diffraction would be a valuable supplement to electron diffraction [10]. In spite of the 10^5 - 10^6 times lower scattering power of X-rays, the intense beam on UPBL9b would probe gas phase reactions over a wider range in q and provide higher spatial resolution, albeit at lower time resolution (1 ps vs 100ps). Simulations have proved the feasibility at pressures ~ 10 torr and exposure times of 10-100 s/image. The S/N ratio should be ~ 10 times greater than in typical liquid experiments. With the higher S/N ratio on UPBL9b, it might be possible to deconvolute the X-ray signals by laser slicing. It works as follows. The sample is initiated by a 2 ps laser pulse and probed by a 100 ps X-ray pulse. Time zero is defined when the laser pulse is in the middle of the X-ray pulse. By collecting images with time delays from -100 ps to +100 ps in steps of 5 ps for example, each image is a composite of a non-excited and excited image. Given that the laser/X-ray jitter is very small (< 1 ps) and that the X-ray pulse-intensity-profile $I(t)$ is known from streak camera measurements, it is possible, mathematically at least, to calculate the instantaneous signal $dS_{\text{inst}}(q, t)$ by a deconvolution algorithm. The feasibility has been tested on $\text{I}_2:\text{CCl}_4$ by Savo Bratos at the University of Paris and the results are promising. Deconvolution will not replace the thrive for shorter X-ray pulses but might rather be a first preparation for a full fledged femtosecond experiment on an XFEL.

1.4 TECHNICAL CONSIDERATIONS

Beamline location and hutches

UPBL9b will stay on ID09 while the high pressure beamline will move to ID15. It seems most cost efficient to leave the experimental setup in the second hutch and use the high pressure hutch as a second optics hutch for micro focusing optics. The ID09A control hutch could be used for sample preparation and a meeting room.

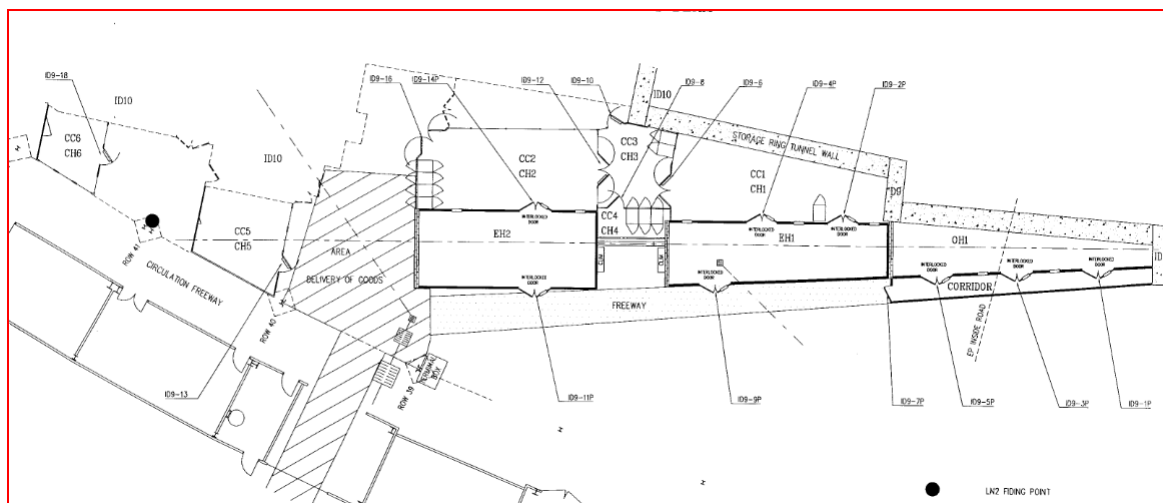


Figure 1. Layout of ID09 as of January 2011.

X-ray source

The 6 m long straight section on ID09 will accommodate two 2.5 m in-vacuum U14 undulators. The fundamental energy of the U14 is tuneable between 18-24 keV ($3 E_f$ between 54-72 keV). The U14 spectrum is shown in Figure 2. The intensity of the tandem undulators at 18 keV is 7.5 times higher than from the U17 today. The U14 has a record 180 periods, which is on the limit of being possible. The vertical divergence will be extremely low, 5.6 μrad (rms) at E_f and 4.3 μrad (rms) at $3E_f$. The low-divergence $3E_f$ beam can be focused efficiently with a platinum coated toroidal mirror at an incidence angle of 1.5 mrad. We expect this high-energy beam for pump-probe experiments to be unique.

The price of doubling the flux with two identical U14 undulators comes at the expense of reducing the available energy range. This point was discussed at the brainstorming and most people support the view that flux is more important than tune ability. The final decision has not been taken and might depend on the importance of the emission spectrometer.

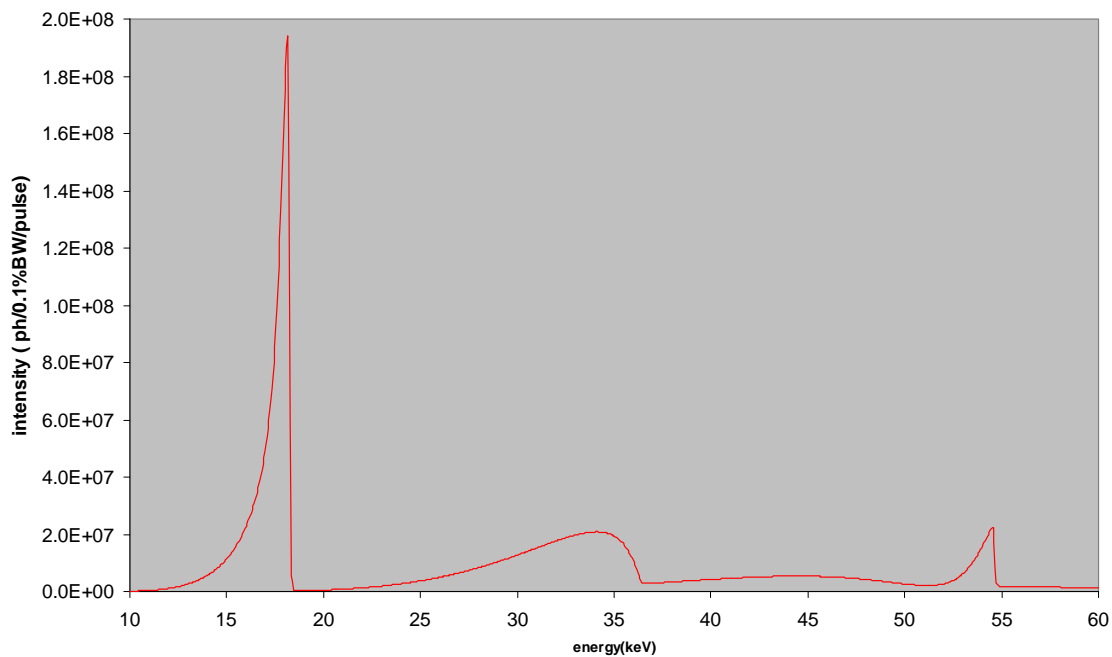


Figure 2. Spectral intensity of two U14 undulators at 6 mm gap. The intensity is calculated for a 5 mA bunch and with primary slits opened to 7 mm H and 0.7 mm V (acceptance of the future toroidal mirror). The integral intensity of the fundamental is 1.2×10^{10} ph/pulse and its bandwidth is 5%.

Toroidal mirrors

The white beam will be focused by two toroidal mirrors, one for the E_f range (18-24 keV) and one for the $3E_f$ range (54-72 keV). The E_f mirror will take the beam at 3.0 mrad, the $3E_f$ mirror at 1.5 mrad. The mirror cut-offs will be 26 and 60 keV respectively with Pt coating. The toroidal shape will be realised by bending a cylindrical mirror to meridian radii R_m of 16.9 and 7.3 km respectively. The sagittal radii r_s are small, 28.6 and 66.0 mm and it might be possible to fit in the two cylinders in one block of silicon to save money and space. The vertical focal size depends primarily on the longitudinal slope errors. Ray tracing with a slope error of $0.55 \mu\text{rad}$ (rms) gives a $40 \mu\text{m}$ round spot for $0.4 < M < 0.5$. By comparison the current spot on ID09 is $105 \times 60 \mu\text{m}$ H x μm V (FWHM). With the new mirrors and the two U14 undulators, the flux density will increase 30 times at 18 keV. The incident power on the mirrors is 970 Watt at 200 mA (primary slits: horizontal gap 7 mm and vertical gap 0.7 mm). The mirror will be preceded by a heatload chopper that will reduce this load down to 50 Watt. The components in the optics hutch are shown in Figure 3.

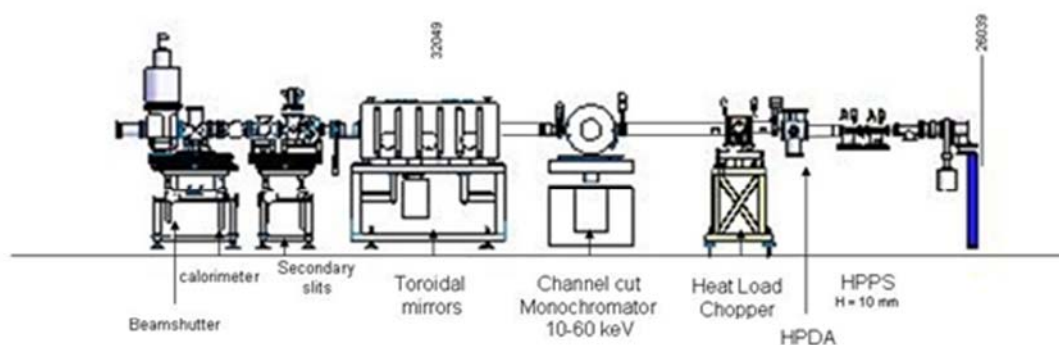


Figure 3. Optics hutch on UPBL9b. The white beam comes from the right.

Monochromators

UPBL9b will keep the existing channel-cut monochromator in the optics hutch on ID09 that produces stable beams between 10-60 keV. The monochromator, which is cryogenically cooled, will be modified to accommodate have two channel-cut crystals, Si (111) for 10-30 keV and Si (220) for 30-60 keV. The blue support table will be replaced by a large concrete block to lower the sensitivity to vibrations from the pumps. The heat load is typically reduced to < 50 Watt by the heat load chopper (but the cryogenic cooling is still needed).

Heat load chopper

This pre-chopper in the optics hutch cuts the white beam into 50 μ s pulses at 1 kHz which reduces the heat load on the downstream optics by a factor of 20. With two U14 undulators, we expect a heat load of 960 Watt (200mA) and the existing wheel design won't work at this power. The solution is to improve the thermal conductivity of the Cu wheel by explosion-binding it to the stainless-steel flange of the ferrofluid feed through, a technique already used for the crutch absorber in the bending magnets in the storage ring. A modified tunnel geometry will allow quick switching between 1 kHz to 3 kHz modes will be particular important for high energy experiments.

Laue-front-end

UPBL9b will use an improved version of the Laue front-end on ID09B, see Figure 4. The critical element is the high-speed chopper which has to be close to the sample where the beam is small from the focusing, in order to chop the beam as fast as possible (265 ns). The first element is a wire monitor for measuring the beam position followed by a (pulsed) ms shutter. The diagnostics chamber contains a PIN diode, a Cyberstar scintillator detector for pulse and time diagnostics and a fluorescence screen with a microscope. The key components are described below.

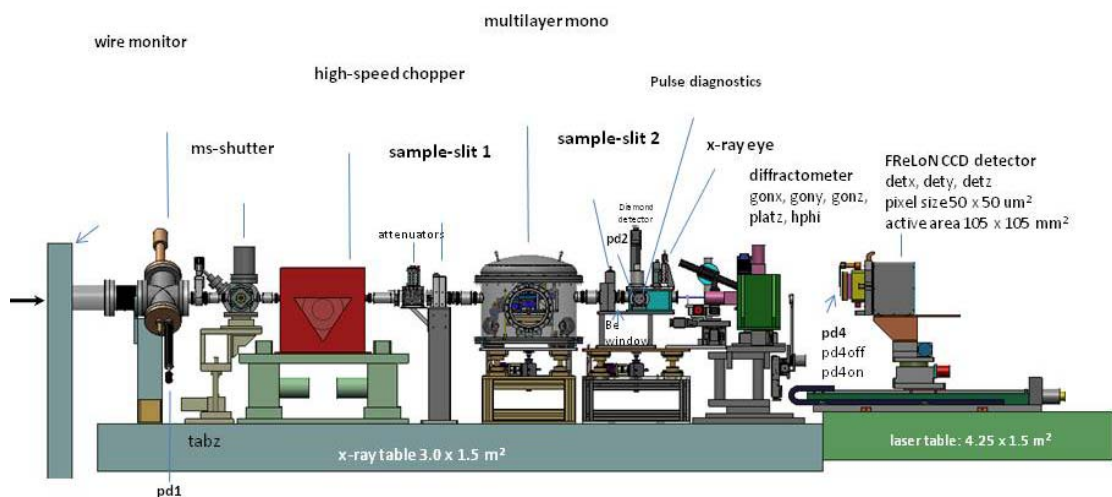


Figure 4a. Experimental table in hutch EH2 for pump-probe experiments. The multilayer monochromator was finished in the summer 2010.



Figure 4b. Laser table with the new picosecond laser and the TOPAS wavelength shifter (white box).

Large-wheel chopper

The triangular rotor in the high-speed chopper on ID09 was upgraded in 2006 to provide a short-pulse mode (200-500 ns) and a long-pulse mode (0.5-20 μ s) in addition to the use of single pulses (100 ps) [10]. In short-pulse mode the beam is led through a semi-open tunnel. In long-pulse mode the beam is passed above the tunnel (tunnel-less chopping). By varying the beam-rotor distance, the open time can be varied continuously which is useful for getting higher pulse intensity in microsecond experiments. Finally 3 kHz pulses can be made by passing the beam above the tunnel where the three rotor tips cut the beam. This is only possible when

the rotor and the beam are very close to each other, typically 10 μm apart, which is the stability limit of the present chopper. If the radius of the rotor is increased from 100 to 150 mm, the time and space tolerances increase to 20 ns and 20 μm which seem feasible in practice. The 3 kHz rotor will be very useful for high-energy experiments where the source output and the detection efficiency are lower.

Laser facility

It is very important to excite the highest possible fraction of molecules without damage the sample. A $(0.1 \text{ mm})^3$ cube of liquid contains about 10^{16} molecules. If we excite 1:1000 molecules, the sample has to absorb 10^{13} photons per pulse. The peak power in a 100 fs visible pulse with 10^{13} photons is ~ 10 MW so it is not surprising that the sample might suffer with femtosecond pulses. We have recently installed a narrow-band-width picosecond laser with 1.6 ps pulses that can be tuned in wavelength from 260 to 1800 nm. The sample preparation lab should provide space for an optical absorption spectrometer.

Detectors

A high speed FReLoN CCD camera is already available on ID09B which has greatly increased the number of time delays that can be collected per day (1400 frames/h for 2 s exposures per frame). Time resolved pixel detectors are now commercially available and with smaller improvement in pixel size and time resolution they will become very important for structural studies on the millisecond time scale. The most obvious application is SAXS/WAXS studies on larger proteins that take longer to move. The perfect linearity of a pixel detector will be a great advantage for the subtraction of *laser-on* and *laser-off* frames as it will increase the accuracy of the normalisation. Time gating a pixel detector is another fascinating option: the left-hand-side of the detection area could be gated to record the non-excited state and the right-hand-side could record the excited state. Recording the excited and non-excited states (quasi) simultaneously the data quality should improve greatly. Finally pixel detectors can already today run in real-time mode about 10 ms time resolution. With smaller improvements in time resolution, pixel detectors will open up the opportunity for probing protein folding and slower mixing reactions activated by diffusion (stop-flow-cell).

Multilayer monochromator

The asymmetric energy spectrum of the undulator harmonics will be made Gaussian with multilayer crystals that are placed 1 m from the sample to improve the stability. The heat load after the two choppers is < 1 W so the multilayer crystals are cooled with water. The multilayers are tailor made for the first (18-24 keV) and third harmonic (54-72 keV) and there are three available bandwidths: 0.1, 1.5 and 3.0%.

The vacuum vessel will also accommodate a water-cooled silicon monochromator with a smaller beam and more stable beam compared to the cryogenic monochromator in the optics hutch. The multilayer monochromator is shown on Fig. 5.

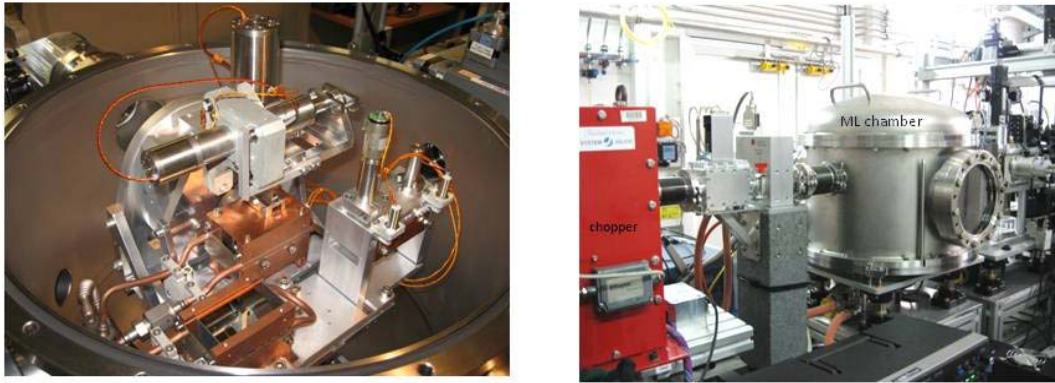


Figure 5. Multilayer monochromator. The interior is shown on the left with the ML crystals in the lower part and the channel-cut in the upper. On the right the ML vacuum vessel show shown downstream to the red chopper chamber.

1.5 REFERENCES

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