# BL43LXU
# RIKEN Quantum NanoDynamics

## 1. Introduction

The bulk of the beamtime at BL43LXU [1] in 2020/2021 was for user experiments, but also included some installation and commissioning of new equipment (see below). The present report will, as usual, emphasize both the changes and the problems at the beamline in an effort to provide a record of progress and to provide useful information to others working to develop SR instrumentation. One notes that the COVID-19 outbreak did impact beamline operation, with user experiments mostly cancelled from mid-April through June of 2020. However, some remote work was carried out, as well as some useful beamline tests and R&D. However, the limitations on international travel had a significant impact and prevented interested user groups from carrying out experiments. One hopes that these restrictions will be relaxed in the near future.

Work at the experimental stations has largely been carried out by members of the Materials Dynamics Laboratory, with assistance on some projects by members of JASRI, RIKEN, and, occasionally, members of the RIKEN engineering team. K. Taguchi also provided part-time assistance and there was also some help from members of the engineering team on specific tasks including the standard start-up of $LN_2$ cooling for the mirror and the high-heat-load (HHL) mono, and, sometimes, beam size measurement and setting up of sample refrigerators.

## 2. Optics hutch and upstream

The upstream components (electron orbit, IDs, mirrors, and HHL mono) were stable during 2020. The orbit-correction protocol operated smoothly, and there were no issues with IDs. The high-heat-load mirror (M1) operated without changes and was stable when used. The BPM (SiC quadrant), just before the sample, is now well integrated into standard operation. Problems with the encoder for th1 were solved by replacing the external (cable-imbedded) electronics.

## 3. Cryomagnet

The cryomagnet was used in one experiment. We will continue to improve the setup and instruct the RIKEN engineering team on how to cool it down.

## 4. Medium-resolution spectrometer

There was one publication based on work using this spectrometer [2]. However, most work during the year used the high-resolution spectrometer.

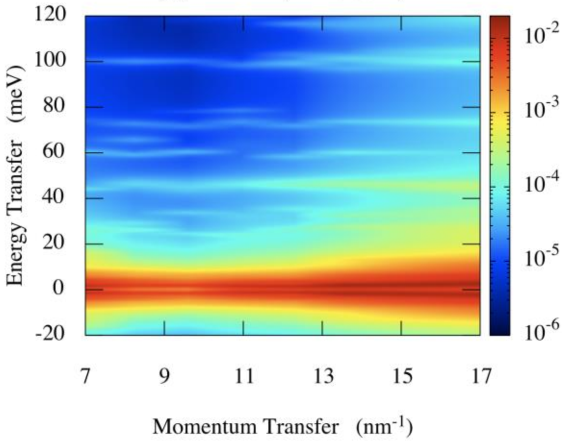
## 5. High-resolution spectrometer

The high-resolution spectrometer operated reasonably over most of the year. The granite plates and airpads remained unscratched after the last polishing by Huber. This may be a result of the increased airflow (higher airpad flight height), but it also just may be a “lucky” year; the reasons for the shifting alignment of the granite plates on the floor are still not understood but might, for example, be related to changes in the water content of the gravel layer under the experimental hall floor. A lot of time was devoted to understanding the cause of some intermittent temperature readout errors (jumps of ~0.01 °C) that occurred on ~hour time scales on some analyzer crystals. This was finally found to be the result of interference of two control programs and fixed.

## 6. Improved resolution functions

An extensive investigation of the samples used to measure resolution functions (PMMA and Tempax glass) was carried out to quantitatively understand the inelastic contributions to the desired elastic response. The phonons in these materials were mapped out over a broad range of energy and momentum transfers. This is now used to deconvolve the phonons from the measured response and generate a smooth approximation to the resolution function (sarf). The work has been published [4]. Figure 1 shows the inelastic scattering measured from plexiglass and Tempax glass; several phonon bands are evident. These are now removed from the measured responses by deconvolution. One also notes that the inelastic intensity near the structure factor maximum is much lower for Tempax glass than for PMMA. Thus, Tempax is a significantly better starting point for measuring the resolution than PMMA.

(a) PMMA (T = 300 K)



(b) TEMPAX (T = 300 K)

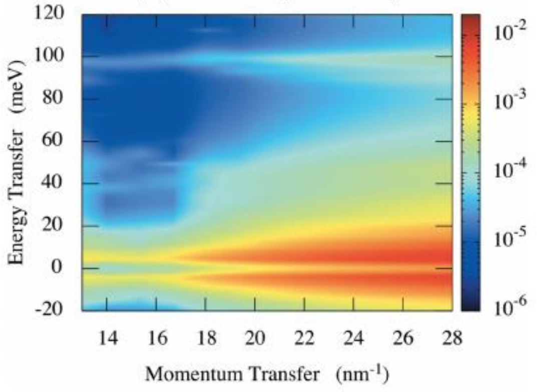


Fig. 1. Inelastic contributions to the responses of (a) plexiglass (PMMA) and (b) Tempax glass over the indicated momentum and energy transfers. The scale is the fraction of the elastic intensity[4].

## 7. Soller screen

The Soller screen setup (see [4]) was modified to with narrower apertures that should provide better S/N (at a cost of reduced S). This was tested and seemed to perform reasonably, allowing measurements above 300 GPa in a DAC. As part of that work, we also performed calculations to confirm the Soller screen performance. An example is shown in Fig. 2. Basically, over some range of angles, the Soller screen performs fully as well as a Soller slit

## 8. Area detector background tests

BL43LXU considers using a pixel area detector for IXS. However, a concern with these detectors is the background rate: the presently

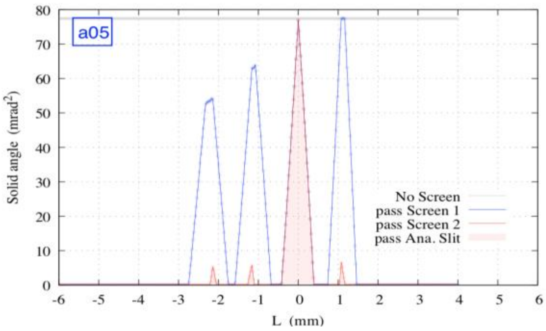


Fig. 2. Calculated acceptance of a Soller screen at a scattering angle of 6.3 degrees. The grey line at the upper part of the plot shows the acceptance L along the beam path, while the red shaded region shows the region that makes it through the Soller screen to the analyzer. A diamond anvil cell, for example, might extend over the region of L=+-2 mm, while the sample will only be ~10 µm thick. Considering the area, it is clear that the Soller screen improves S/N by a factor of 10 or more.

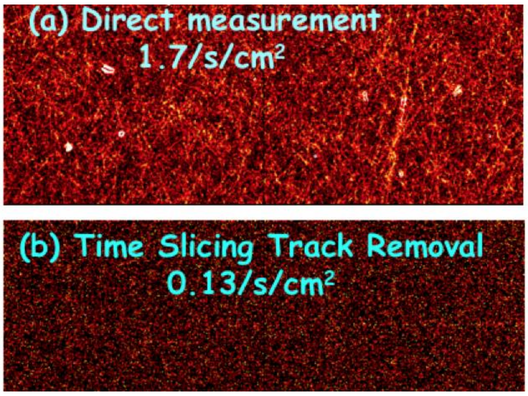


Fig. 3. Using time-slicing to reduce the background from cosmic ray muons in an area detector (Pilatus 100K). Simple processing can reduce rates to ~0.1/s/cm$^2$ while more advanced processing is expected to reduce it further.

used CdZnTe detectors (Hamamatsu) have background rates that are very low, ~0.001/s/channel (1 channel is 2x2 mm$^2$, so this is 0.025/s/cm$^2$), and we would like to match this, or do even better, with an area detector. First tests were carried out using a CdTe 300K Pilatus detector from Dectris. However, even after the removal of track or cluster events (e.g., from cosmic-ray muons; see figure 3) the best background achieved was only ~0.13/s/cm$^2$, that is, about 5 times that of the present detectors. This is under investigation. It is hoped (and expected) that an upper level discriminator will reduce the background by about one order of magnitude.

## 9. Mode interactions in water

The first published work [5] using the previously demonstrated sub-meV resolution [6] that was optimized for liquid investigations appeared during this time. The work showed that what had previously been interpreted as an indication of transverse dynamics in liquid water was actually the result of a hydrodynamically expected interaction between the scattering from quasi-elastic and phonon modes in water (see Fig. 4). This demonstrates some of the differences between the atomic dynamics of liquid and solids, and changed the picture of the onset of positive dispersion.

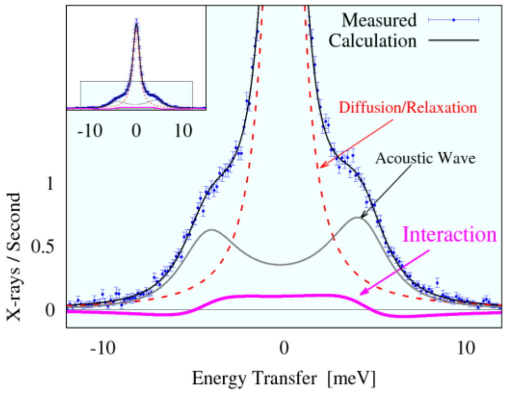


Fig. 4. Interaction contribution in the spectra of water. A careful investigation of a previous theory from the 1970s shows the term and the dramatic improvement of the fits (with no increase in the number of free parameters), and confirms that it is present and important..

Alfred Q. R. Baron & Daisuke Ishikawa
Materials Dynamics Group, Photon Science Research Division, RIKEN SPring-8 Center

**References:**

[1] Baron, A. Q. R. (2010). *SPring-8 Inf. Newsl.* **15**, 14. http://user.spring8.or.jp/sp8info/?p=3138 and Baron, A. Q. R. (2010). In *Synchrotron Light Sources Free. Lasers Accel. Physics, Instrum. Sci.*, edited by E. Jaeschke et al. (Springer, Cham), pp. 1643–1757.
See also http://arxiv.org/abs/1504.01098

[2] Ishikawa, D. & Baron, A. Q. R. (2021). *J. Synchrotron Radiat.* **28**, 756.
https://doi.org/10.1107/S160057752100179X

[3] Baron, A. Q. R., Ishikawa, D., Fukui, H. & Nakajima, Y. (2019). *AIP Conf. Proc.* **2054**, 20002.
https://aip.scitation.org/doi/abs/10.1063/1.5084562.
See also https://arxiv.org/abs/1807.03620

[4] Ishikawa, D. & Baron, A. Q. R. (2021). *J. Synchrotron Radiat.* **28**, 804.
https://doi.org/10.1107/S1600577521003234

[5] Ishikawa, D. & Baron, A. Q. R. (2021). *J. Phys. Soc. Jpn.* **90**, 83602.
https://doi.org/10.7566/JPSJ.90.083602

[6] Ishikawa, D., Ellis, D. S., Uchiyama, H. & Baron, A. Q. R. (2015). *J. Synchrotron Radiat.* **22**, 3.
https://doi.org/10.1107/S1600577514021006