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Report:

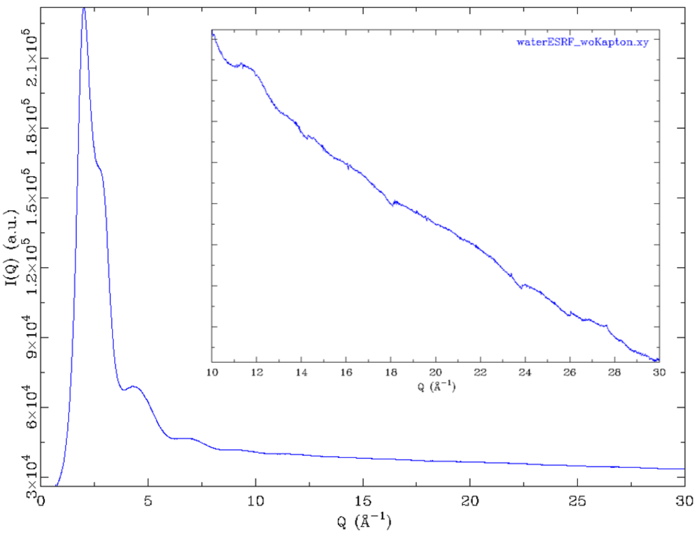
The beamtime was carried out using the novel Pilatus 2M CdTe. In order to achieve a minimum $Q = 0.6$ Å^{-1}, a flying beamstop had to be implemented at the beamline. The CdTe detector was offset. Unfortunately the beamline was haunted by some technical issues, so that the overall measurement time was almost reduced to half. Initial problems with tailing effects of the primary X-ray beam from upstream slits were followed by safety problems and ESRF technicians had to intervene and restart the safety system on the beamline as the mechanical brake of the detector mount was not working as it should. Nevertheless, we collected good data on the solvation shells as well as on complementary data on restructured water in pores. Data analysis is however far from finished as we ran into some new problems with the CdTe, which have not been reported before. For this, I will give below a short wrap-up of the issues, so that data collection and processing with the CdTe detector can be improved for upcoming beamtimes and other users.

<u>Collimator</u>

The beamline is rather new and therefore not everything can be perfectly in place. However, it seems to happen every now and then with non-standard setups that the long collimator tube, which rather loosely lies on lead pieces, is easily touched and moves a few microns, which requires a tedious re-alignment. Hopefully, a more fixed positioning is available in the future.

<u>Glitches in data after radial integration</u>

We appreciated a lot the CdTe detector with its very astonishing signal-to-noise ratio at large Q. The radially integrated data showed several glitches, in particular at large Q, see the inset of the figure showing data on water in a Kapton capillary. These glitches become very obvious due to the smooth curves of the diffraction signal of water (it would be the same for any other liquid and such glitches are observed for powders as well, but less obvious). Data was integrated both with Fit2D and Dioptas, giving the same result. We had a long discussion with the authors of Dioptas/pyFAI, also including our beamline scientists. We came to the



result that data corrections (polarization, flatfield, absorption) play a very important role when treating the CdTe data, in particular the solid angle and polarization corrections. The gaps in between the individual sectors of the detector cause the glitches and the solid angle correction seems to amplify it. We were told that also the detectors edges always cause glitches when running the radial integration over the edges; although we are still puzzled by this and do not really understand their origin.

However, this shows that software development is a very crucial piece for getting excellent data from the best technical equipment nowadays. It might be worth a thought whether the software crew to provide software to ESRF users should be strenghtened in the future. It is astonishing that even nowadays the bottleneck in a quick analysis and publication of our beamtime data is the fundamental radial integration of detector images, which seems to be unsolved currently in the scientific community for the high-qualitly data of the new CdTe detectors.

Flatfield

The performance of the CdTe detector changes over time. Directly after our beamtime a new flatfield was taken by the beamline scientists, which was significantly different from the one which was provided during our beamtime. We do not know how “old” the one was, which we had used to correct our data. It might be quite important to provide current flatfields to users, who are looking for tiny signals, highly diluted systems, weakly scattering samples, etc.; i.e. more important than maybe initally pointed out by the manufacturer’s experience.

Data collection mode

Previous Perkin Elmer detectors are often run in accumulation mode to improve signal-to-noise ratios. The Pilatus CdTe detector is a single photon counting detector, which enables a very small noise level.

The detector control is embedded in the spec environment of the control computers and it is possible to change the collection mode of the CdTe detector from “accumulation” to “single photon counting” within the LIMA submenu of the control computer. Throughout our beamtime we were provided with only vague information about how the detector actually works and only on the last day and having a look at the detector manual jointly with all beamline scientists, we discussed the working principle and how we actually measured. The latter was not really clear to part of the beamline scientist crew, which therefore could not advise us during our beamtime to the desired extent.

The CdTe detector works in single-photon counting mode and therefore, the big question was, why it is possible to change its collection mode in the ESRF software implementation from “accumulation” to “single photon counting” and what in fact is changed in the collection mode. Is it the way images are summed or is it the statistical error bars that can be modified?

Conclusion

We are well aware that the CdTe detectors are new, and most likely part of their performance is unknown and also not reported by the manufacturer. Therefore, the above points are meant as general suggestions on how to improve the data quality of CdTe detectors to really be able to use their full capability and e.g. not to be limited by flatfield accurateness or unawareness of data collection modes. The radial integration seems to be a more general issue that due to our experiments with liquids was clearly observed and right now prevents any data analysis from our beamtime.

We have an upcoming beamtime midth of February and hope to be able to discuss with beamline scientists how to treat our data from the last beamtime. It is in general publication-quality, just the radial integration screws it currently. It was suggested for our upcoming beamtime to collect data with different detector positions (moving the detector by ca. 20 pixels) to lessen the glitches after radial integration. However, the motors of the detectors move slowly so that detector movements will cost more time than we spend on actual data collection. Moreover, if we have to move the detectors in order to remove the glitches, this kills the possibility to run high-quality in-situ studies with high time resolution.

We are still troubled whether there might not be a work-around the glithces purely by improving the radial integration to obtain data without glitches. Strengthening the ESRF software crew to tackle such questions might be worth a thought as radial integration is of general importance to all users.

We are happy to contribute to the development of the best data collection strategies and sharing our thoughts on the radial integration in order to get the most out of the new CdTe detectors for all of us.