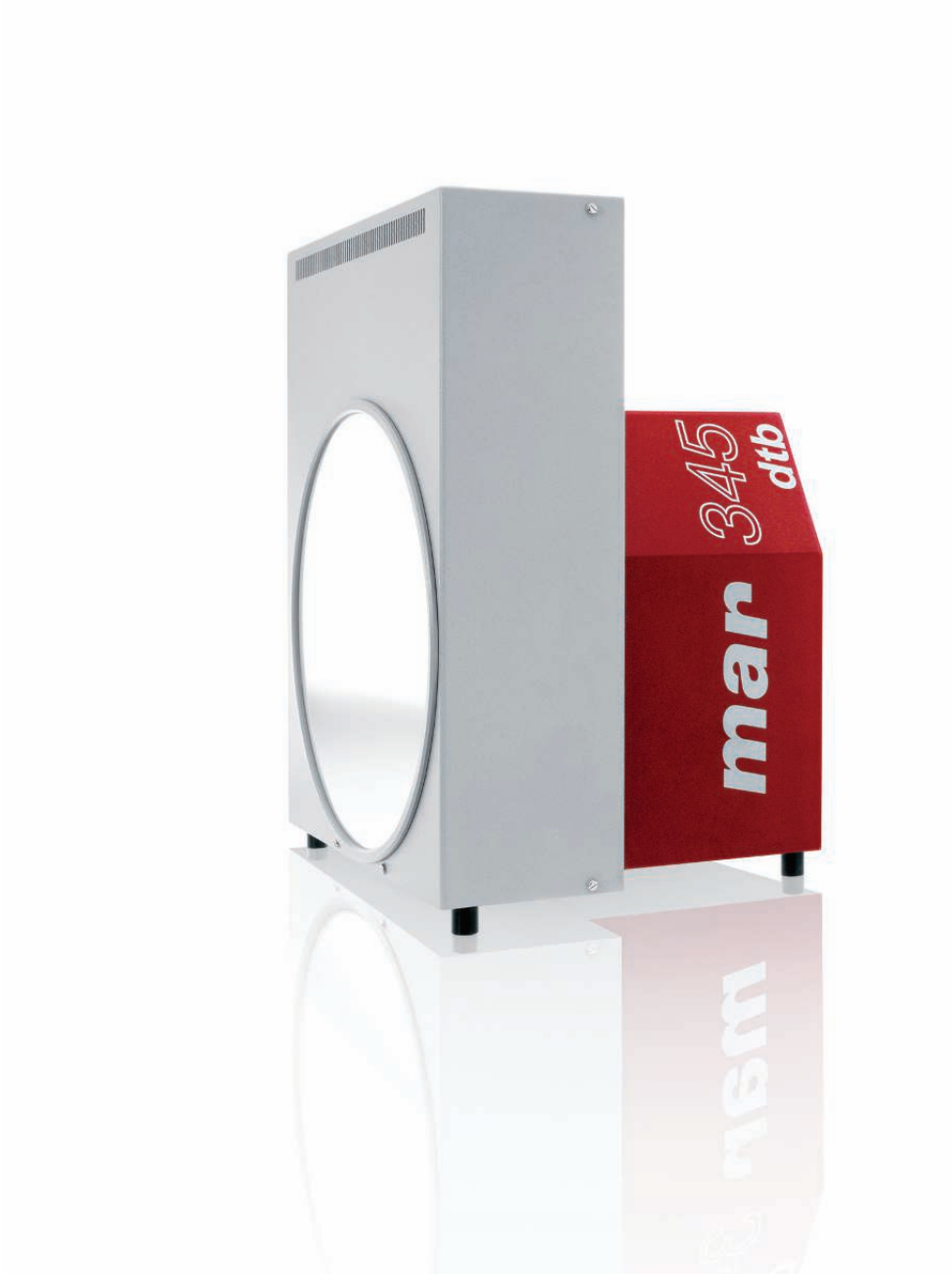

Comparison of the fast and fine read-out modes of the mar345 S image plate detector

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1. Introduction

The mar345s is a new variant of the well known mar345 image plate detector. Today, many detectors are used on conventional X-ray sources for crystal screening and crystal characterization while full data collection has moved to synchrotron sites that deliver so many more X-ray photons. The typical detector requirements for this type of in-house work are:

- very sensitive and very low noise to keep exposure times reasonably short
- fast read-out to quickly see the results and estimate the quality of diffraction
- low purchase price and low costs-of-ownership

The detector technologies competing with the image plate detectors are solid-state detectors like the CCD technology, the pixel detectors and CMOS detectors. None of the available detectors is perfect. They are either noisy (CMOS), small (pixel- & CCD-detectors) or expensive (pixel- & CCD-detectors). Even worse, while those detectors can be read-out quickly in the range of seconds to milliseconds, one typically has to expose the sample 2 to 10 times longer for getting similar results as with the mar345 image plate detector. On conventional X-ray sources with typical exposure times of >= 5 minutes per degree of data for protein crystals, the amount of X-ray photons required to produce a given signal on the detector is the time limiting step in obtaining results, not the read-out time!

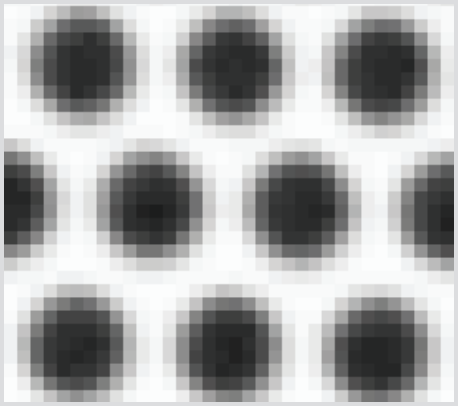
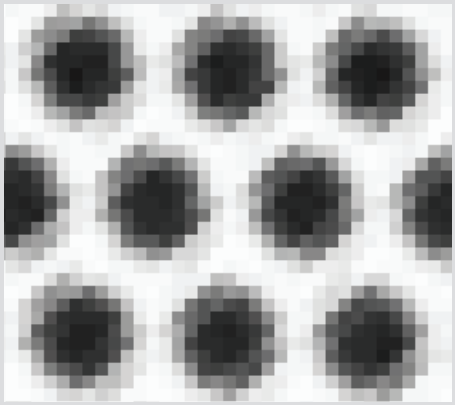
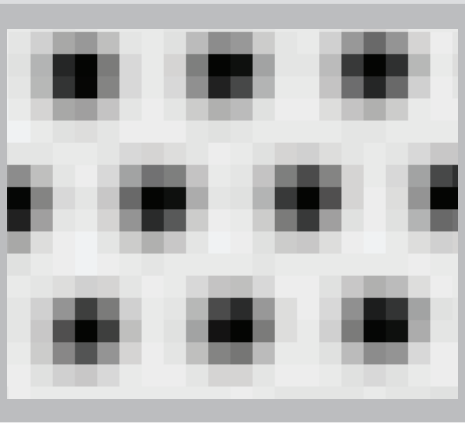
In this regard, the image plate detector comes close to the ideal detector for conventional X-ray sources if it was not for the rather long read-out cycles of 35 to 110 seconds, depending on scanned area and pixel size. This is why the new mar345s detector has been made considerably faster to shorten the time to evaluate the crystal quality during screening work. This has been achieved almost without sacrificing data quality.

The four fast new scan modes implemented in the mar345s detector replace the scan modes with 100 µm pixel size at 345, 300, 240 and 180 mm plate diameter, respectively. The average pixel size in the transformed Carthesian image is 150 µm. While the read-out time itself is approximately 50% of the corresponding time for the standard 150 µm scan modes, the overhead times for positioning the reading head and erasing the plate are the same. This gives a typical speed gain of **35%** for the most typical use of the 345 mm diameter scan. In the user software you will see the resulting image as soon as the read-out is finished, so you can start inspecting the image before the total cycle time is over. The following table gives and overview of the read-out and total cycle times:

Read-Out and Cycle Times

Scanned diameter	180 mm		240 mm		300 mm		345 mm	
Scan mode	Fine	**Fast**	Fine	**Fast**	Fine	**Fast**	Fine	**Fast**
Read-out time [sec]	18	**9**	30	**15**	47	**23**	58	**30**
Total cycle time [sec]	34	**27**	48	**34**	66	**43**	80	**53**
Fine -> Fast	-21 %		-29 %		-35 %		-35 %	

In order to estimate the loss of quality of the new fast scan modes compared to the standard fine 150 µm scan modes, we have irradiated perforated plates with a flat X-ray field. The perforated plates feature defined holes of 0.2 mm and 1.5 mm diameter at regular intervals of 1.0 mm and 1.75 mm, respectively. The results are shown in the next figure. It can clearly be seen that the spatial resolution of the fine 150 µm scan mode is superior to the one of the new fast scan mode. But spot separation is still very good and unless the quality of the X-ray beam becomes very good (i.e. very low divergence with synchrotron beam) or the cell axes become very long the effects are seemingly negligible.

	Fine 150 µm scan mode	Fast 150 µm scan mode
Perforated plate 1.75 / 1.5 mm The holes have a diameter of 1.5 mm and a distance of 1.75 mm from each other.		
Perforated plate 1.00 / 0.2 mm The holes have a diameter of 0.2 mm and a distance of 1.00 mm from each other.		

2. Data collection and processing

2.1 Small molecule data

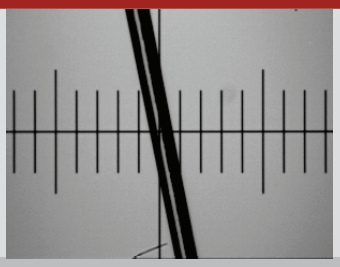
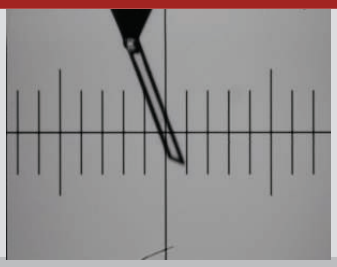
To estimate the quality difference between the new fast scan mode and the fine scan mode data were collected on a marµX2G system consisting of a:

- marµS micro-focus generator running at 50 kV/600mA with a Cu anode
- mar345S image plate detector
- mardtb goniostat

Crystals from a small molecule - ammonium bitartrate - were used to collect data at:

- 80 mm distance crystal-to-detector giving 1.44 Ang. resolution at the edge
- 5 deg./image
- 72 images (i.e. 360 deg. of data)
- constant exposure time (6 s/image)

Data were processed using the automar program suite. The space-group of the bitartrate crystals is P $2_1 2_1 2_1$.The unit cell axes are a=7.6, b=7.8, c=11.1 Ang..

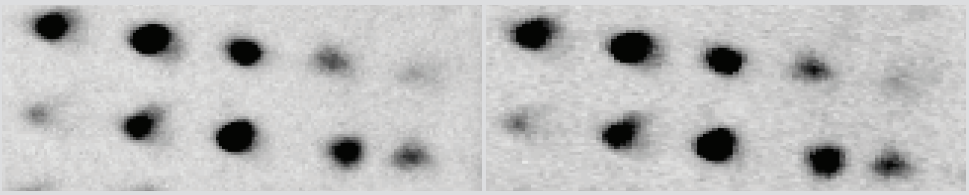
	Crystal 1		Crystal 2	
Crystal				
Mosaicity [deg.]	0.6^0		0.3^0	
Size of crystal W x H x L [µm]	150 x 130 x 2000		30 x 60 x 500	
Scan mode	**Fine**	**Fast**	**Fine**	**Fast**
# unique reflections	106	107	117	116
Multiplicity	9.8	9.9	9.8	9.7
Rsym	4.23	4.17	3.12	3.54
Rpim	1.25	1.31	1.10	1.20
<Intensity>	120.113	106.365	46.623	40.510
<I/σ>	48.6	46.4	45.6	45.1

2.2 Protein data

Data from a protein molecule - lysozyme - were collected on a rotating anode generator with a mar345s image plate detector mounted on a mardtb goniostat (courtesy of I. Korndörfer, Crelux GmbH) at:

- 200 mm distance crystal-to-detector giving 2.3 Ang. resolution at the edge
- 1^0/image
- 180 images (i.e. 180^0 of data)
- constant exposure time (300 s/image)

Data were processed using the automar program suite. The space-group of the lysozyme crystals is P 4_32_12.The unit cell axes are a=78.5, b=78.5, c=37.7 Ang.. The mosaicity of the crystal was approx. 0.8^0.

Scan mode	Fine	Fast
Pattern from image # 10		
# unique reflections	5311	5357
Multiplicity	11.1	11.2
Rsym	4.34	3.61
Rpim	1.33	1.14
<Intensity>	24907	28341
<I/σ>	13.3	14.5

Surprisingly, the data collected in the new fast scan modes are slightly better than the ones in the fine scan mode. There is no other explanation for this than a deterioration of the crystal during the course of data collection. In this case, the fast scan mode data were collected first. Nevertheless, the experiment proves that the fast scan mode does not visibly deteriorate the quality of the data obtained from proteins.

3. Conclusion

The small molecule data of the new fast scan modes show a slightly decreased average intensity. The loss is around 12% as compared to the fine scan mode. Since the read-out is twice as fast for the fast scan mode this loss of efficiency seems surprisingly low! The typical data quality indicators (Rsym, Rpim, I/σ) of the fast scan mode data come very close to those of the fine scan mode and show the same behaviour. While, clearly, the overall quality of the fine scan modes is slightly better, for practical use this seems to be negligible. The better quality of the protein data obtained with the new fast scan modes are somewhat inconsistent with the results from the small molecule data, but we blame the crystal for this finding.

The data collected here suggest, that - unless the ultimate data quality is the primary goal - users should be using the new fast scan modes as their default. This is particularly true for screening samples, where users rarely look at processed data but rather want to get a quick overview of the diffraction power of their sample. The new fast scan modes will provide the same answers to these questions as the slower fine scan modes do but in significantly shorter time!