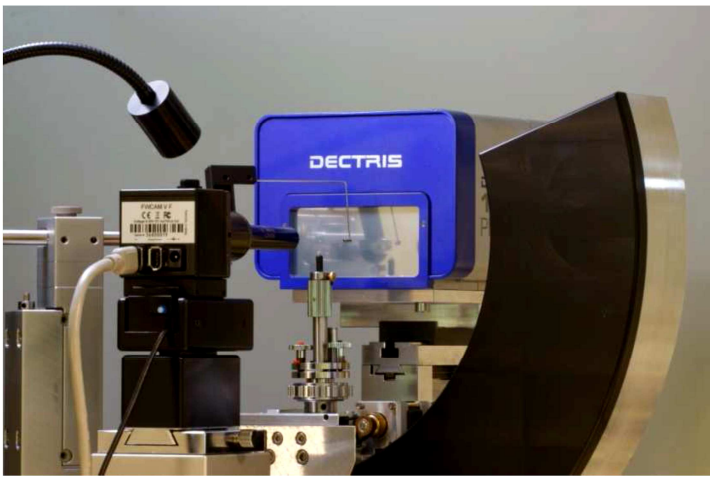
LABNOTE

STOE STADIVARI - FIRST RESULTS WITH A NEW DIFFRACTOMETER SYSTEM

CHARACTERISTICS

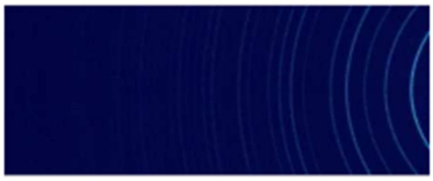
The new **STOE STADIVARI** with an Open Eulerian Cradle has been combined with a DECTRIS Pilatus 100K detector to a unique diffractometer system. The combination of the goniometer's high precision and the outstanding performance of the detector yields to impressive results.



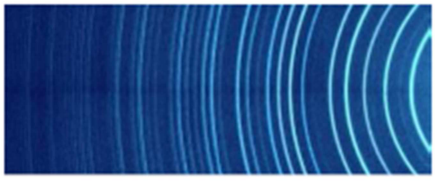
As a first test some powder frames with LaB_6 have been collected to prove the specifications of the Pilatus 100K.

In a second step data from a single crystal (Ca Tartrate) has been collected with different exposure times to determine how fast a data collection can be performed. The influence of the experimental time on the quality of the data collection has also been a point of interest.

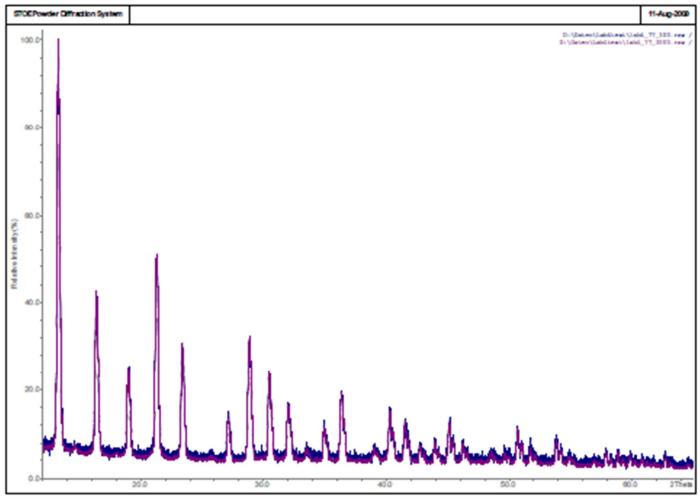
LaB_6 EXPERIMENT



LaB_6 exposed for 300 sec.



LaB_6 exposed for 3000 sec.



The comparison of the two measurements carried out at different exposure times shows the excellent performance and noise behavior of the Pilatus 100K detector. No influence of the exposure time on the width of the reflections can be noticed. The long-time measurement results in a better statistics of the background and shows impurities in the LaB_6 sample a little bit better than the short-time measurement.

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Ca-TARTRATE EXPERIMENT

A well diffracting crystal has been measured at different exposure times to determine the quality of the different data sets. The measurements have been performed as 'shutterless' measurements consisting of 24 runs with a scanning angle of 1° and exposure times of 1s, 5s and 30s per frame. The detector has been positioned at 40° in 2θ and at a distance of 47 mm to the crystal. The maximum 2θ value reached has been 80°. For the comparison the data have been cut at 60° in 2θ. The measurement has been performed at 298 K.

Exposure time / frame	1 s	5 s	30 s
Experiment time	**0.4 h**	**1.7 h**	**9.9 h**
Mean I / sigma	6.38	16.63	43.05
Completeness	100%	100%	100%
Redundancy	8.84	8.84	8.83
N (I > 4 sigma)	2330	2576	2667
N	2737	2737	2737
R (int)	0.0688	0.0505	0.0412
R (sigma)	0.1070	0.0378	0.0143
R1*	0.0401	0.0286	0.0246
R1 (all)*	**0.0532**	**0.0316**	**0.0255**
wR2	0.0724	0.0708	0.0660
GooF	0.945	1.061	1.127
Highest Peak	0.37	0.38	0.41
Deepest Hole	-0.56	-0.54	-0.53

** All hydrogen atoms were found in the difference Fourier map and have been refined.*

The comparison shows that the final data quality is not affected too much by the use of a short exposure time. This result may be different if a weak scattering crystal will be used. In this case longer exposure times will yield in a higher mean I/sigma and may probably visualize effects which can be overlooked.

Conclusion

The combination of the STOE STADIVARI, the Open Eulerian Cradle and the Dectris Pilatus 100K in combination with the X-Area software results in a very flexible and powerful instrument to fulfill almost any need of a crystallographer. The extreme low noise of the detector and the excellent point spread function allow long time exposures as well as very short exposure times. The new STADIVARI allows due to its modularity various sample stages, up to the Open Eulerian Cradle.