Table 2. Speed up of calculation as dependent on execution methods

Execution methods	1 CPU core from DASH GUI	1 CPU core from MDASH	2 CPU core from MDASH	4 CPU core from MDASH	8 CPU core from MDASH	12 CPU core from MDASH	16 CPU core from MDASH
Time required to find 1 correct solution/sec	1113	1144	470	240	108	116	126

with 2x Intel Xeon E560, 2.4 GHz processors (8 real cores). We wanted to know whatever the utilization of hyper-threading and virtual 16 processors can give any benefit. The speed tests were done for the methylergometrin maleate structure. Results are summarized in Tab. 2.

The use of optimized SA parameters can clearly make a difference between finding a solution or not finding solution at all, especially for high DOF structures. The use of Mogul bias looks a bit problematic - for non usual structures with atypical geometry (ixazomib with boron atom) it can give less benefit than for common molecules. The time required for solution is reduced proportionally to number of true CPU used for calculation. The use of virtual hyper-threading CPU gives no benefit and slow-down the calculations. For methylergometrin maleate the combination of optimized SA parameters, Mogul bias used and parallel processing on 8 CPU give up to 47x speed up in comparison to standard calculation setup.

1. E. A. Kabova, PhD thesis, University of Reading, 2016.

This work was supported by the Czech Science Foundation (GA ČR) project, Grant No. 16-10035S.

Session VIII, Wednesday, June 20

CL4

NEW DEVELOPMENTS IN MICROFOCUS SOURCES FOR X-RAY DIFFRACTOMETRY

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Many applications in the field of X-ray analytics require an X-ray beam with high flux density at the sample position. Examples for these applications are single crystal diffraction, small angle scattering or microdiffraction to name but a few. The ideal source for diffractometry combines a device, that produces a microfocus X-ray beam of a size of below 50 µm, with a perfectly shaped high-reflectivity X-ray optics like multilayer mirrors, that are able to focus or collimate the beam to the sample or detector position.
In this contribution we will be presenting the latest developments of this kind of solution. Our family of air-cooled Incoatec Microfocus Sources deliver collimated beams with a divergence of below 0.5 mrad or focused beams with sizes down to about 100 µm with a flux of up to $5x10^8$ ph/s. Most of these sources are integrated in standard instruments. More and more they are also successfully integrated in customized set ups for in-situ measurements of crystal and thin film growth.

We will be showing some examples in the field of X-ray diffractometry and SAXS, that were not long ago only possible with synchrotron or rotating anode sources.

L23

EXPERIENCE WITH POWDER X-RAY DIFFRACTOMETER BRUKER D8 ADVANCE: AUTOMATIC DIVERGENCE SLIT, VARIABLE COUNTING TIME DATA COLLECTION

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The importance of careful sample preparation and data collection in powder X-ray diffraction studies have been described on several previous occasions. Laboratory instruments normally have favoured configuration which is used for a wide range of experiments. In many laboratories, custom and/or time pressure, rather than a considered approach, often determine the data collection strategy [1]. Before collection of powder diffraction pattern, it is a good idea to know what information you might get out of it and consider the appropriate data collection strategy. Parameters which can be considered include angular range, step size, counting time, wavelength etc. For example, the qualitative phase identification generally requires only relatively small 2 range containing the strongest reflections of the sample, the meaningful Rietveld refinement (i.e. for the purpose of quantitative phase analysis) requires high quality data measured to small *d* values [2]. In this presentation, two techniques which can improve the data quality in Bragg-Brentano geometry, will be presented. The conventional Bruker D8 Advance diffractometer with the Cu*K*á tube and the Lynx Eye XE detector was used for the data collection.

The application of the *automatic divergence slit* (ADS) (also called Theta compensating slit) ensures that the irradiated sample length is kept equal over a measured range of 2 . This in turn leads to higher diffracted intensities in middle and higher area of 2 . As is shown in Fig. 1, this is the main advantage of ADS slit in comparison to the traditional fixed divergence slit (FDS). Moreover, the application of automatic divergence slit may prevent the undesired effect of beam overflow at low diffraction angles, which may occur when large fixed diverge slit (typically 1° or larger) is used.

The diffracted intensity in conventional X-ray diffraction patterns decrease with the increased diffraction angle. The main physical factors which cause this variation include the drop atomic scattering factors, thermal vibrations and the Lorentz-polarisation factor. *Variable counting time* data collection strategy (VCT) may significantly improve the statistic quality of data at the middle and high diffraction angles.

1. R. D. Hill & I. C. Madsen, in *Structure Determination from Powder Diffraction Data*, edited by W. I. F. David, K. Shankland, L. B. McCusker & Ch. Baerlocher (Oxford University press), 2002, pp. 98-117.
2. J. K. Cockcroft & A. N. Fitch, in *Powder Diffraction Theory and Practice*, edited by R. E. Dinnebier & S. J. L. Billinge (Cambridge: The Royal Society of Chemistry), 2008, pp. 20-57.

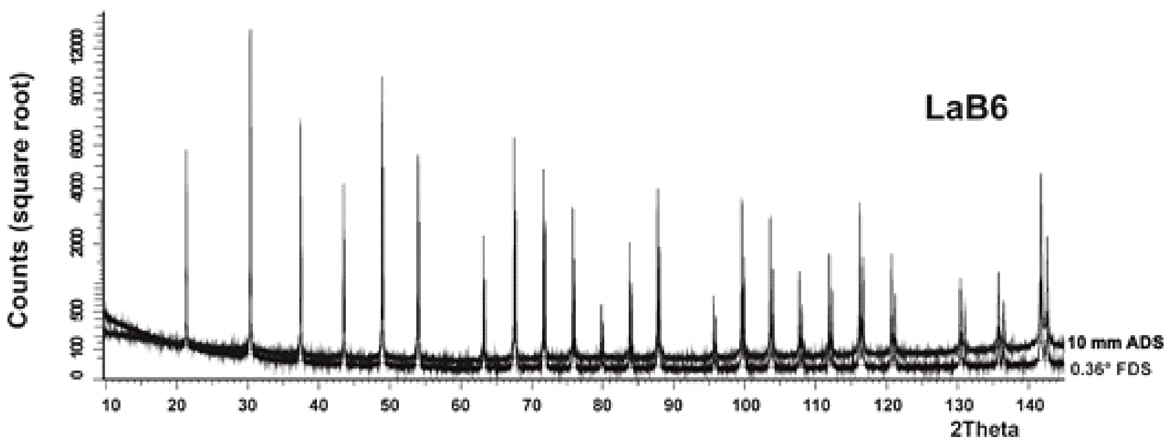

Figure 1. Comparison of diffraction patterns of LaB_6 collected with automatic and fixed divergence slits.