Quantum RX

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Report
Resolution of the PLANET

Introduction

The **planet** is the high resolution portable X-ray diffractometer from xplorex. With 'high resolution' we mean that the attainable resolution with the planet is comparable to a standard laboratory system and thus by far the best resolution hitherto obtained with a portable system.

In this note we demonstrate the attainable resolution with the planet with a normal measurement on normal commercial LaB_6.

Experimental

About 1g of the as-received powder was pressed into the sample holder (so-called front loading). The prepared specimen was mounted in the diffractometer and measured. Because the **planet** uses a reflection geometry, sample preparation is not critical even for heavy absorbers like LaB_6. The measurement parameters are summarized in Table 1.

Parameter	Value
Range	
Start Angle (°2θ)	19.3
End Angle (°2θ)	101.3
Step size	Variable; The **planet** has predefined step sizes
Angle of incidence (°)	14.47
Integration time	120s / data point (the measurement comprises 14 times 640 data points)
Total Measurement time	32 minutes
Diffractometer settings	
High Tension	30 kV
Emission Current	0.65 mA
Tube anode	Cu
Focus dimensions	40µm diameter
Take off angle (°)	8
Beam divergence (°)	1.25
Specimen dimensions	7mm diameter; 2mm thickness
Spinning frequency	0.5 Hz
Optical path	Seemann – Bohlin based
Focusing circle radius	160mm
Detector	Dectris' Mythen 1D solid state linear detector
Identification software	Match! From Crystal Impact
Reference database	Crystallographic Open Database

Table 1 Measurement parameters for LaB_6 sample

The diffractometer settings are constant for the **planet**. The operator can choose the measurement range and the integration time for optimal results and ease-of-use.

Results

Figure 1 shows the complete diffraction pattern we recorded from the as received LaB_6 specimen.

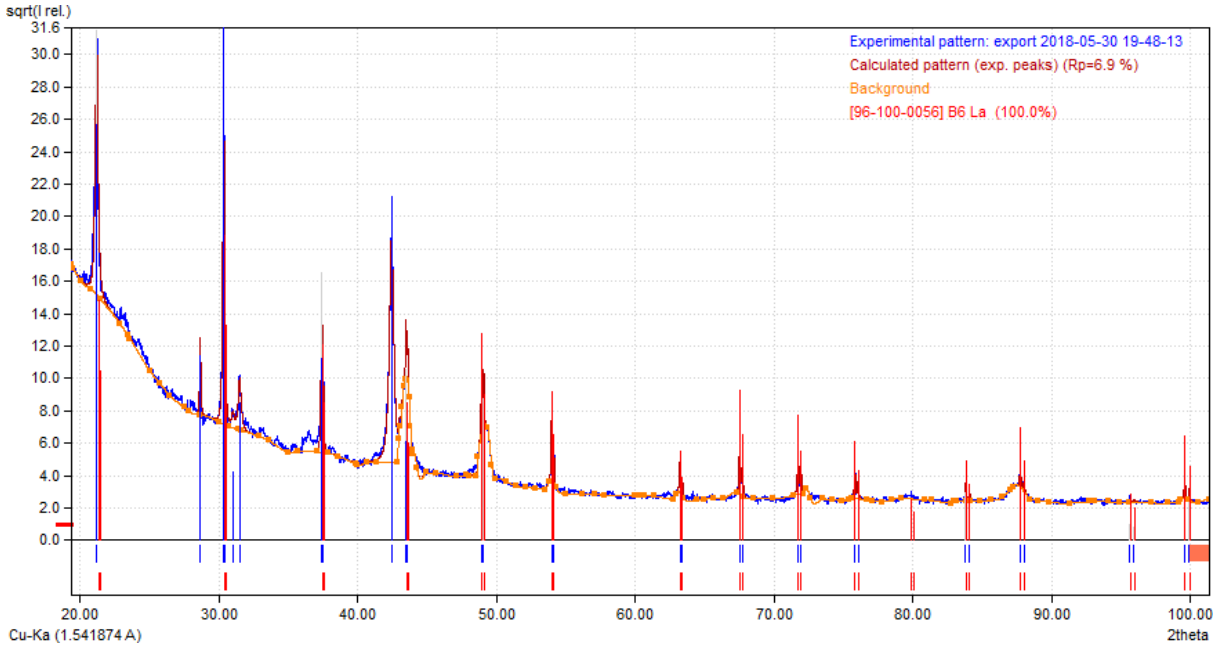

Figure 1 Diffraction pattern from commercial LaB_6

To assess the attainable resolution of the **planet** we performed careful profile fitting on each observed reflection from LaB_6 and we reported the FWHM. The results of this exercise are shown in Table 2.

Table 2 Full Width at Half Maximum for LaB_6 reflections

Scattering angle (°2θ)	FWHM (°2θ)
21.357	0.198
30.384	0.109
37.441	0.092
43.506	0.084
48.956	0.070
53.987	0.079
63.217	0.083
67.546	0.084
71.744	0.091
75.842	0.089
83.843	0.102
87.789	0.087
99.639	0.083

As can be seen the FWHM is below 0.11° for all reflections except the first one (0.20°), where the beam path is significantly shorter. The length of the beam and the focus dimensions determine the attainable

resolution for any reflection. This confirms that the attainable resolution for all reflections is best in class, for any portable XRD in the market.

Comparison with a laboratory-based system

Because we used commercial LaB_6, we had to validate that this material is suitable for resolution measurements. To this end we measured both our commercial sample and a standard material (NIST 660a) on a laboratory-based system. These measurements are given by the Red (commercial) and Black (standard) curve in Figure 2.

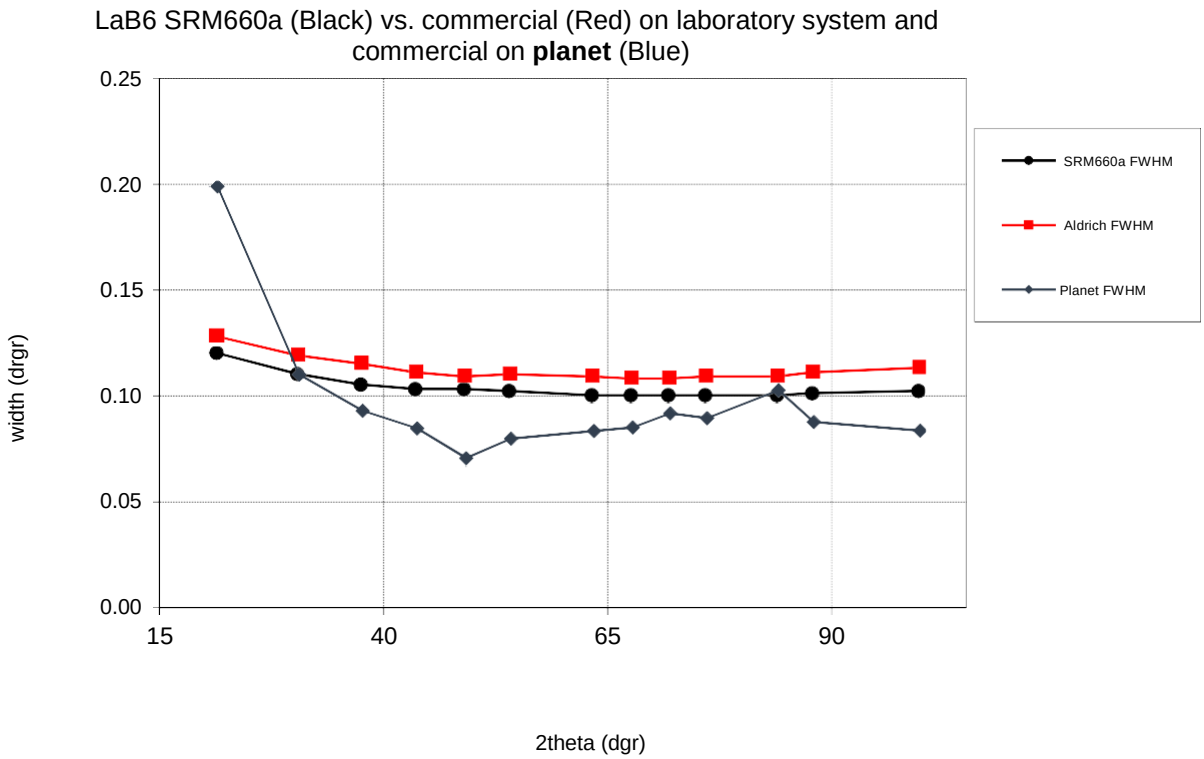

Figure 2 FWHM measurements on laboratory system and planet

In the same graph we plotted the FWHM values we measured on the **planet** (Blue curve). We determined the FWHM by profile fitting in "Match!" from Crystal Impact. Please note that, although we measured the commercial sample with the **planet**, the FWHM values of all but the first reflections are even below the ones measured on the standard sample with a normal laboratory-based diffractometer! Moreover, we see the best resolution between 40 and 65°2θ, where it matters most, because generally the peak density is highest in that range.

Conclusion

The attainable resolution of the planet compares well to the attainable resolution of a standard laboratory-based instrument. The attainable resolution of the planet is best in class among currently available portable X-ray diffractometers.