

Evaluation of Unisantis XMD 300 Polycapillary Optic Parallel Beam Diffractometer using NIST Line Position Standard (SRM 660a)

Abstract

Determination of precise peak positions is critical to any powder diffraction data related to qualitative and quantitative phase identification.

This study evaluates the peak positions obtained with Unisantis Polycapillary Optic Parallel Beam Diffractometer using the NIST SRM 660a Instrument Line Position Standard.

It was observed that the peak data obtained with Unisantis XMD 300 are within $\pm 0.01^\circ$ of the certified line positions.



Introduction

Peak positions or line positions in any x-ray diffractogram are very important in any diffraction experiment. The ability of a powder diffractometer to provide precise and accurate line positions establishes the quality of the instrument.

The Standard Reference Material 660a has been specially developed by National Institute of Standards to determine how precisely an x-ray diffractometer can determine the line positions from a diffraction pattern.

Inaccurate and faulty line positions are bound to adversely affect the results obtained in applications like phase identification, stress analysis and unit cell indexing.

In the present study NIST SRM 660 was used to evaluate the performance of Unisantis XMD 300, a polycapillary optic parallel beam x-ray diffractometer. The peak positional accuracy was determined using the standard reference material.

Table 1. System Configuration	
Unisantis XMD 300 Diffractometer	
X-Ray Tube	50W Air cooled
Incident Beam Optics	Polycapillary Half-lens
Tube Voltage	45 kV
Tube Current	1 mA
Detector	Position Sensitive Detector
Sample Stage	Standard sample stage with laser alignment

The diffractogram obtained for NIST SRM 660a, using the above instrumental configuration is given in Fig.1.

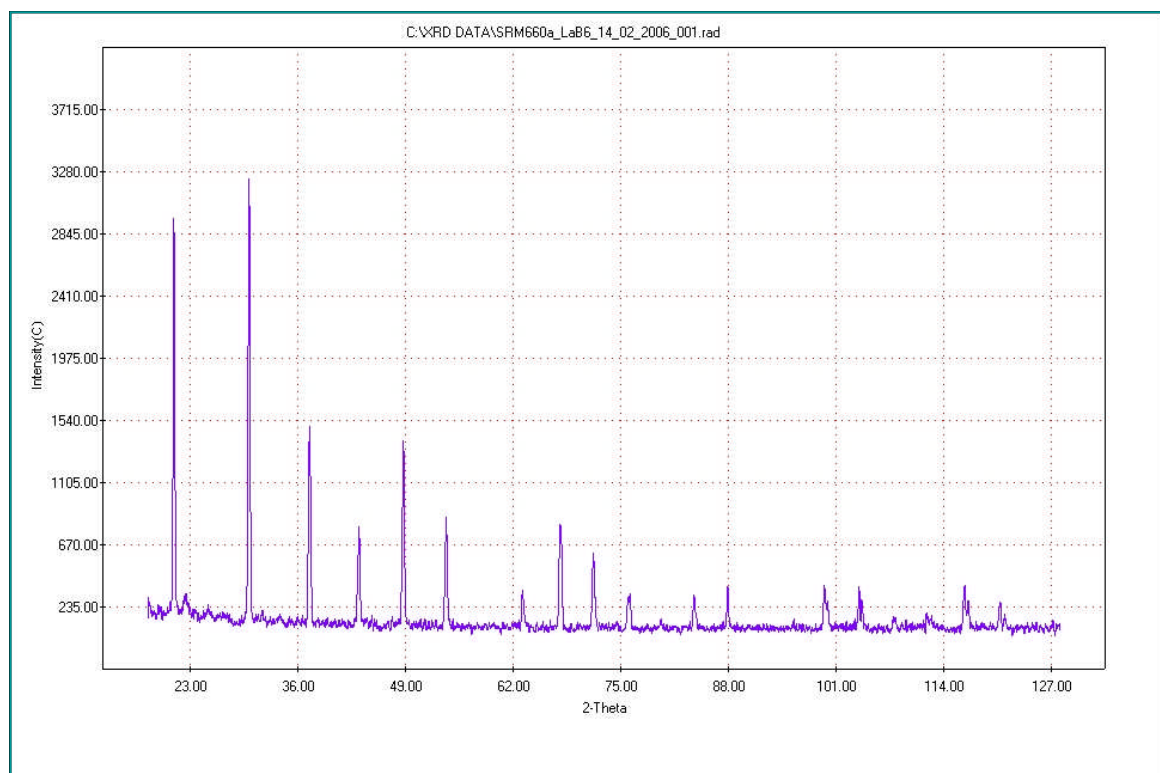


Fig 1. XRD Pattern of NIST SRM 660a obtained from Unisantis XMD300

Results

The line positions (2 theta values) found by the Unisantis XMD 300 Diffractometer were subtracted from the line positions certified by NIST.

The difference was then plotted against the certified line positions. The results of this 2 theta difference plot are shown in Figure 2.

It may be noted that the line positions were obtained from the raw data of the sample.

The data obtained from Unisantis XMD 300 shows a very small deviation from zero.

The largest deviation was found to be 0.01045° . This difference very well agrees with the value suggested in literature.

The quality of this data is excellent considering the fact that the data has not been corrected for any of the errors known to be generally associated with powder diffraction experiments

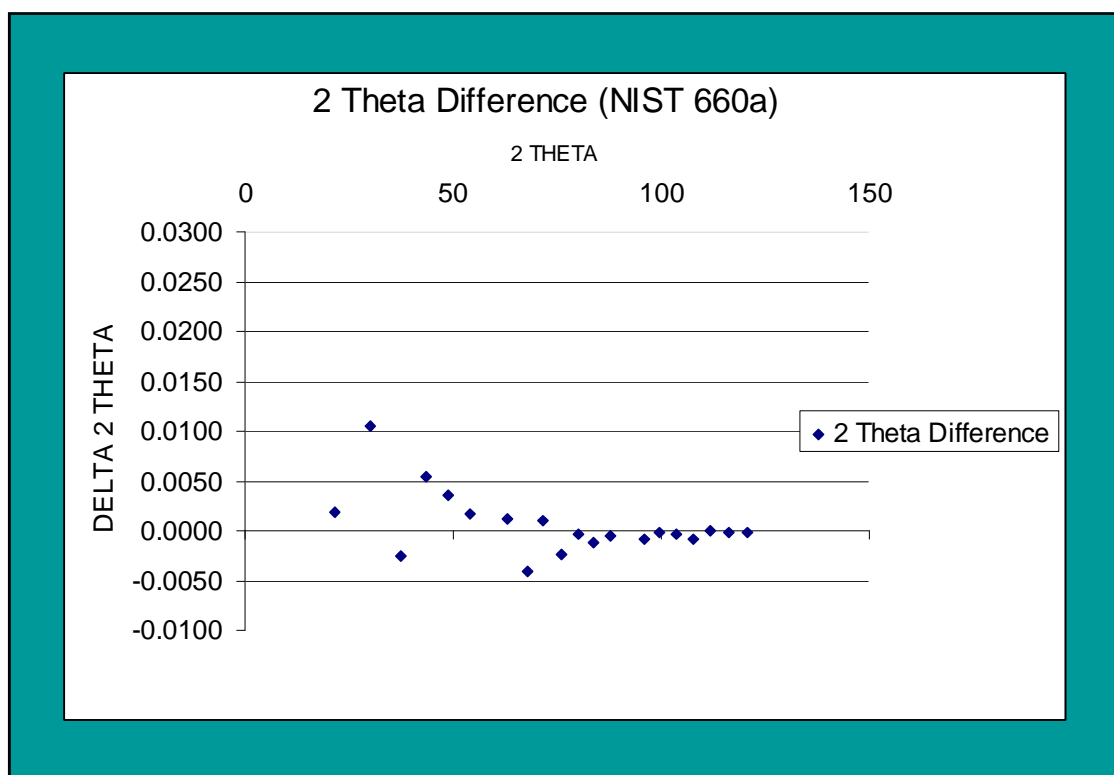


Figure 2. $\Delta 2\theta$ versus 2θ for SRM 660 a as obtained on Unisantis XMD 300

Conclusions

The present study demonstrates that Unisantis XMD 300 Polycapillary Optic Parallel Beam Diffractometer provides precise, uncorrected line positions . Thus, the data provided by Unisantis XMD 300 is highly suitable for all X-ray diffraction studies such as phase identification, stress analysis and unit cell indexing.

The quality of diffraction data obtained using a low power tube is exceptionally good.

Hence the user can be confident that any major shift in the line position in the X-ray diffraction pattern is not due to the instrument.

It may be noted that due to its parallel beam geometry the data provided by XMD is without any instrumental errors known to be associated with conventional powder diffractometers such as sample displacement error, sample transparency errors etc.,

Company profile

Unisantis Europe GmbH is a global leader in development and manufacturing of innovative X-Ray analytical instrumentation, complete solutions and software for structure and elemental analysis using proprietary Polycapillary optics known for best beam collimation. Success in research has enabled Unisantis Europe GmbH to develop new cutting -edge X-ray technology, applications and products for the market. Our products have particular applications in material characterization, life science and industrial analysis.

Unisantis instruments incorporate a new range of user benefits, including transportability and multifunctionality all comprised in compact, bench top, user friendly, environmentally safe and low energy consumption equipment.

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