

## BRAGG-BRENTANO<sup>HD</sup>

# Setting a new standard for high-quality powder diffraction data... and more

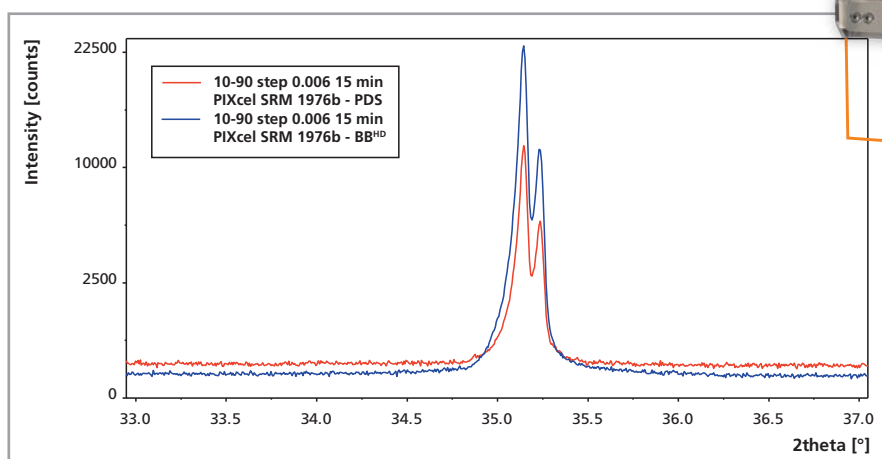
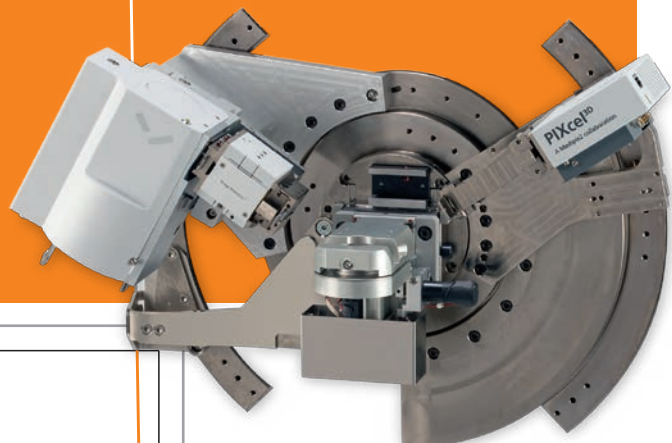


Figure 1: Comparison of two data sets recorded on NIST SRM1976b. For both measurements, the optics settings were chosen to create matching peak shapes. The red data set was recorded with a conventional programmable divergence slit (PDS) set to  $1/4^\circ$ , the blue data set (recorded with a Bragg-Brentano<sup>HD</sup>) shows a higher intensity and lower background.

### Introduction

With the introduction of Bragg-Brentano<sup>HD</sup>, PANalytical again sets a new standard for recording high-speed, high-quality powder diffraction data, with the following key features:

- Excellent monochromatization of the radiation from the X-ray source, with the following benefits:
  - Higher intensities than with the commonly used divergence slits and beta filters
  - A smooth, featureless background profile along the full  $2\theta$  range without the usual artifacts of the 1D Bragg-Brentano setup, allowing reliable identification of trace phases, and less chance of misinterpretation by inexperienced users
  - Improved detection limits, leading to better quantification of trace phases and/or amorphous components
  - Better low-angle performance
  - Minimal excitation of fluorescent radiation from the sample
- Extends the range of applications of the powder diffractometer without the need for additional modules
  - Analysis of thin films by grazing incidence diffraction and X-ray reflectivity
  - Nanoparticle size, shape and size distribution analysis by small angle X-ray scattering (SAXS)
  - Micro-spot analysis
- Compatible with all PANalytical's multipurpose powder diffractometers, both on new systems and already installed ones

### Summary

Bragg-Brentano<sup>HD</sup> is the latest addition to PANalytical's extensive portfolio of PreFIX optical modules. It combines the high-speed datacollection speed of one- and two-dimensional detectors with the data quality of traditional powder diffractometers equipped with a receiving slit.

In addition, Bragg-Brentano<sup>HD</sup> can also be used for thin film and nanoparticle analysis.

### Background/relevance

In the quantitative analysis of mixtures, detection of trace phases and amorphous components is a difficult task, requiring a low background in the measurement and long data collection times.

Bragg-Brentano<sup>HD</sup> improves the sensitivity, without compromising the data collection time.

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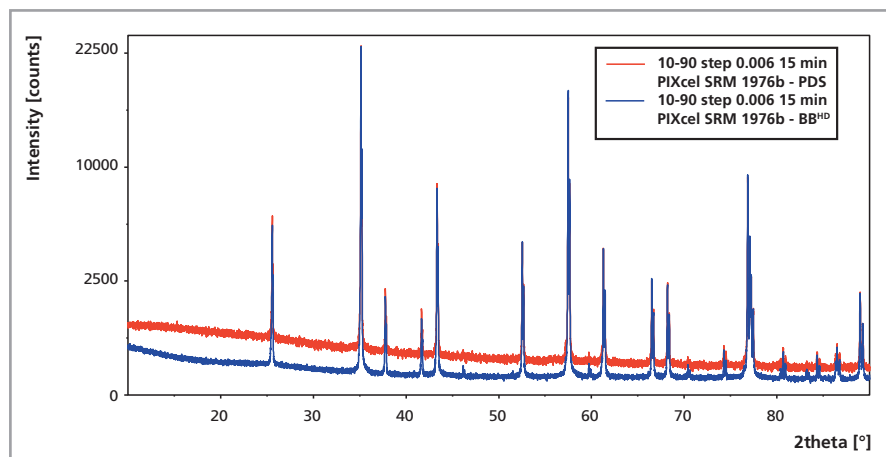


Figure 2: Same sample as in Figure 1. A scale factor of 1.96 was applied to the data recorded with the divergence slit in order to match the tops of the strongest peak. In the measurement recorded with Bragg-Brentano<sup>HD</sup>, the peak-to-background ratio is 3 times higher, and the overall background is lower, making the visibility of weak reflections (e.g. the (202) reflection near 46 ° 2θ) better.

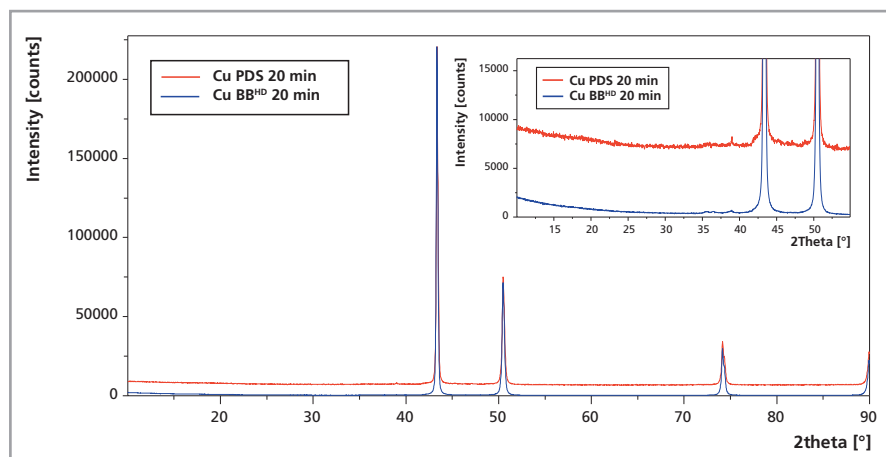


Figure 3: A measurement with slit optics and a beta filter (red) on a Cu-rich sample shows a very high background due to fluorescent radiation from the sample. With Bragg-Brentano<sup>HD</sup> (blue), this fluorescent background is completely absent. The insert shows a detailed view of the background. The presence of a beta filter-induced absorption edge in the slits measurement is visible close to 42 ° which is absent in the Bragg-Brentano<sup>HD</sup> data set. In the latter, the residual Kβ peak (near 39 °) is much lower, and one can also see tiny peaks from a contamination in the sample between 35 ° and 37 °, which only become visible in the scan with slit optics after a much longer scan time.

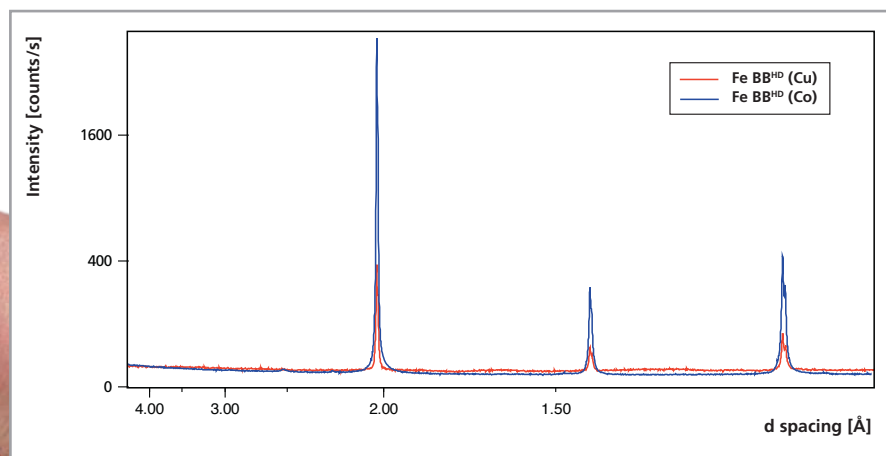


Figure 4: A high concentration of Fe in a sample is known to result in an increase of the background level. Also here, a good peak-to-background ratio (red) can be obtained by optimizing the lower level of the pulse height discriminator. Alternatively, a 1D diffracted beam monochromator can be used. For iron-rich samples, the use of cobalt radiation is a much better choice. The peaks are more intense, and an excellent peak-to-background ratio is achieved with Bragg-Brentano<sup>HD</sup> setup for Co radiation (blue scan).



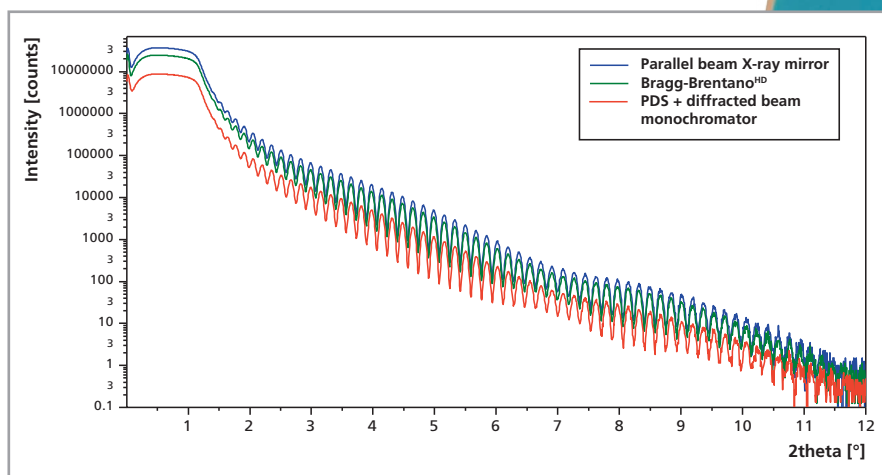


Figure 5: Comparison of reflectograms from a 50 nm thick iridium layer deposited on top of a silicon substrate. Excellent data can be obtained with Bragg-Brentano<sup>HD</sup>; there is no need for a separate diffracted beam monochromator or a parallel beam mirror.

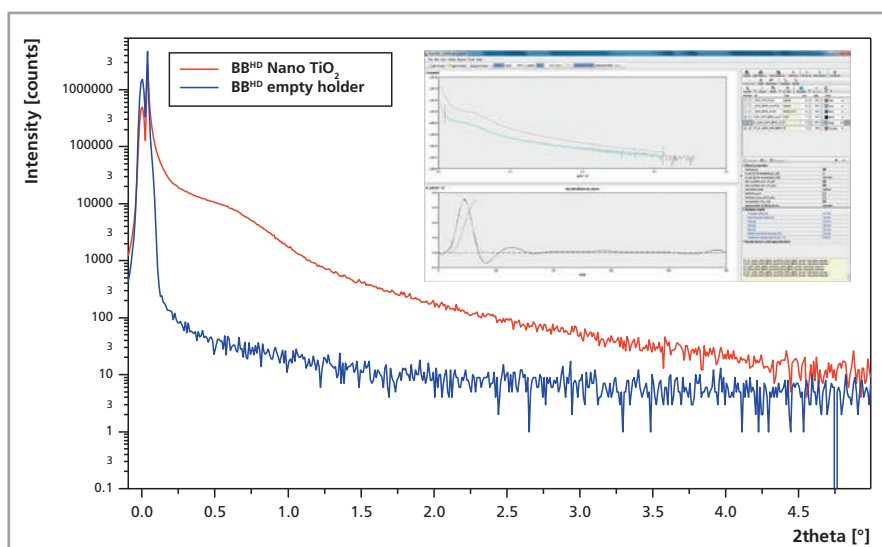


Figure 6: Small angle X-ray scattering (SAXS) data collected using Bragg-Brentano<sup>HD</sup>. In red, the scattering curve from the sample and in blue the background from the holder. In the inset, the analysis of the data performed with the EasySAXS software is shown, resulting in a particle size of 4.4 nm, as expected for this sample.

### Bragg-Brentano<sup>HD</sup> specifications

|                              |                                                                |
|------------------------------|----------------------------------------------------------------|
| Bragg-Brentano <sup>HD</sup> | Incident beam PreFIX module                                    |
| Used with                    | Cu radiation (version for Co radiation available upon request) |
| Energy resolution            | <450 eV                                                        |
| Cu $K\beta$ suppression      | Remaining $K\beta$ <0.2% $K\alpha$                             |

### Conclusions

Bragg-Brentano<sup>HD</sup> sets the standard for the fastest recording of powder diffraction data with a low and smooth background. Bragg-Brentano<sup>HD</sup> maximizes the throughput in the laboratory, while minimizing the chance for misinterpreting trace features in the data.

The same optic can be used for high-quality measurements on thin films (layer thickness) and nanomaterials (particle size distribution analysis)

Bragg-Brentano<sup>HD</sup> is available for new PANalytical instruments, and can be retrofitted to already delivered multipurpose diffractometers equipped with PreFIX.

## Global and near



### PANalytical

PANalytical is the world's leading supplier of analytical instrumentation and software for X-ray diffraction (XRD) and X-ray fluorescence spectrometry (XRF). The materials characterization equipment is used for scientific research and development, for industrial process control applications and for semiconductor metrology.

During the last decade PANalytical has added a variety of other analysis techniques to their product portfolio. Optical emission spectrometry (OBLF GmbH, Germany), pulsed fast thermal neutron activation (Sodern, France) and near-infrared (ASD Inc.) capabilities together with XRD and XRF can provide customers with tailor-made analytical solutions for the characterization of a wide range of products such as cement, metals, nanomaterials, polymers and many more.

PANalytical's headquarters are in Almelo, the Netherlands. Fully equipped application laboratories are established in Japan, China, the USA, Brazil, and the Netherlands. PANalytical's research activities are based in Almelo (NL) and on the campus of the University of Sussex in Brighton (UK). Supply and competence centers are located on two sites in the Netherlands: Almelo (development and production of X-ray instruments) and Eindhoven (development and production of X-ray tubes) and in Boulder, USA (development and production of near-infrared instruments). PANalytical is active in all but a few countries of the world. This worldwide sales and service network ensures unrivalled levels of customer support.

The company is certified in accordance with ISO 9001 and ISO 14001.

Visit our website at [www.panalytical.com](http://www.panalytical.com) for more information about our activities.

PANalytical is part of Spectris plc, the productivity-enhancing instrumentation and controls company.

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