



Spec Sheet XRD 30

Göbel Mirrors

Properties and Potentials

The introduction of curved multilayer x-ray mirrors signified a quantum leap in the beam quality achievable with in-house x-ray sources. Named after Herbert Göbel, who presented mirror designs, characteristics and applications at the 1995 Denver X-ray Conference, the Göbel Mirrors were awarded the R&D 100 award for 1996.

Due to its ability to make highly-parallel x-ray beams, the parabolically-shaped Göbel Mirror quickly became the most widely used. The parallel beams from it removed the traditional limitations of the Bragg-Brentano geometry for powder diffraction and thin film investigations.

Elliptically-shaped or flat mirrors for focusing or Bragg-Brentano beam conditions also remain important optical components for special applications in XRD, single crystal diffraction (SCD) or small angle X-ray scattering (SAXS).

Since their discovery, continued advances in the understanding and fabrication of the mirrors have made it possible to tune mirror performance exactly to the analytical requirements. Therefore, Bruker AXS, in close cooperation with Incoatec, is able to provide mirrors for routine applications as well as special designs for cutting-edge experiments.



Fig. 1: D8 ADVANCE with Göbel Mirror and Flip-Stick sample changer.

In contrast to conventional monochromator crystals, Göbel Mirrors are synthetic crystals whose properties are defined by complex multi-layers which are deposited on silicon or glass substrates under ultra-high vacuum conditions. To shape the mirror, one of two methods is used. The most common is to carefully bend a silicon substrate, either before or after the multilayer structure is deposited, depending upon the application. For highly-demanding thin film requirements, the mirror can be fabricated using a pre-shaped quartz substrate, a Bruker AXS & Incoatec proprietary technology.

Typically, the layer thicknesses of the mirrors are an order of magnitude larger than those of the commonly-used monochromator crystals. Therefore, the 'Bragg angles' for the diffracted beams are an order of magnitude smaller, typically near 1.5°. As a consequence, the reflectivity and the beam divergence of the beams conditioned by a Göbel Mirror are larger than the ones from a monochromator, which yields a monochromatized beam without sacrificing intensity. The ability to monochromatize the beam from the X-ray source is limited to suppressing unwanted $K\beta$ -radiation and the high-energy Bremsstrahlung spectrum. However, compared to instrumental setups with filters only, the background scattering is reduced, which results in better peak-to-background ratio and hence better data quality.

For line focus applications, four commonly used types of Göbel Mirror can be distinguished:

- Multipurpose Göbel Mirror – the all-rounder
- High-resolution Göbel Mirror – dedicated for thin film applications
- Phase ID Göbel Mirror – for powder diffraction in reflection geometry
- Focusing Göbel Mirror – for powder diffraction in transmission geometry

Table 1. Current technical specification of the different types of Göbel Mirror.

Göbel Mirror type	Substrate	Coating	Figure error ³⁾ rms ⁴⁾ [deg]	Total divergence [deg]
Multipurpose	Bent Silicon wafer	WSi ₂ -C	< 0.005	≤ 0.033
High-resolution	Prefigured SiO ₂	WSi ₂ -C	< 0.001	≤ 0.028
Phase ID	Bent Silicon wafer	W-C	< 0.005	≤ 0.07
Focusing ¹⁾	Bent Silicon wafer	W-C	< 0.005	≈ 0.21 ²⁾

All parameters are given for Cu radiation.

For line focus FF tubes 8 x 0.4 mm, 6° take off, 40 μm projected focus width the typical cross-fire is: 0.4 mrad = 0.023 deg (100 mm source to mirror center).

¹⁾ primary focal length $f_1=120$ mm, secondary focal length $f_2=350$ mm

²⁾ convergence angle

³⁾ deviation from ideal shape

⁴⁾ root mean square

The multipurpose Göbel Mirror (fig. 2) is suited for most applications; it is a real all-round talent. Additionally, this mirror is the ideal component to be combined with a traditional Bragg-Brentano instrument. On demand, the user can switch between BB-geometry and parallel beam conditions without realigning the instrument.

The full potential of the high-resolution mirror is utilized when investigating thin films by X-ray Reflectometry (XRR), High-Resolution X-Ray Diffraction (HRXRD), or In-Plane Grazing Incidence Diffraction (IP-GID). If the mirror is used as a pre-conditioner for a channel cut monochromator (fig. 3), a boost of X-ray beam intensity is generated in comparison to a traditional configuration of spot focus X-ray tube and stand-alone channel cut monochromator. Furthermore, the wavelength purity of the beam after the channel cut is drastically improved, so that High-Resolution X-ray Diffraction (HRXRD) investigations with faster data acquisition and better data quality can be performed.

The Phase ID Göbel Mirror is the best choice when the typical investigations are on powder samples which are measured in reflection geometry (fig. 4), for qualitative and quantitative phase identification. By dedicated modification

of the mirror parameters, the beam properties are tuned for improved matching of powder diffraction requirements. The beam from the mirror is wider and has an adjusted divergence, which leads to a larger illuminated area, more intensity, and better counting statistics. The Phase ID Göbel Mirror also provides parallel beam conditions (fig. 4) and allows an easy switch to Bragg-Brentano geometry without need for realignment.

With the growing interest in weakly-scattering samples like polymers or pharmaceuticals, high-flux X-ray optics have become increasingly important. One possibility for increasing the flux is to produce a focused beam, as is done with the Vario1, a Johansson type Germanium monochromator that provides pure $K\alpha_1$ -radiation. For comparison, a focusing Göbel mirror provides $K\alpha$ -radiation only, but with higher beam intensity. Therefore, as long as peak overlaps in the measurements play a secondary role, a focusing mirror in particular in combination with a state-of-the-art 1-dimensional detector is an attractive X-ray optic for high-throughput foil or capillary transmission (fig. 5). Obviously, the focusing Göbel Mirror provides push-plug capability for an alignment-free switch to Bragg-Brentano geometry.



Fig. 2a: Multipurpose Göbel Mirror beam path – XRPD in reflection and transmission on the same sample or in the same sample batch.

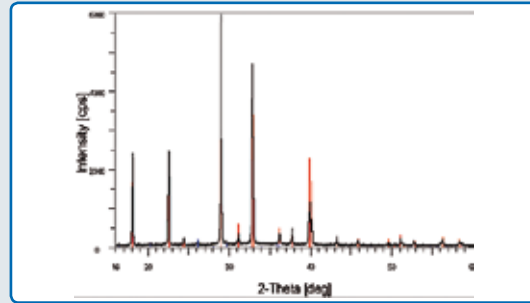


Fig. 2b: Measurement result recorded on Nitrammit in reflection geometry at 0.1% relative humidity; Cu-radiation, parallel beam Göbel Mirror, 5° axial Soller slit, Hot Humidity system, 0.12° diffracted beam Soller slit, and scintillation counter. The red sticks indicate the peak positions taken from ICDD pattern 47-0867.

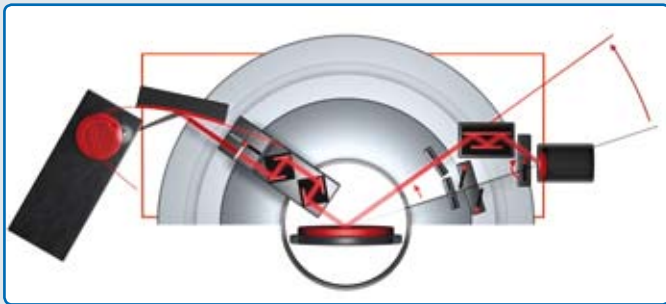


Fig. 3a: High Resolution Göbel Mirror beam path - Göbel Mirror used as a pre-conditioner for a 4-bounce channel cut monochromator in a HRXRD set up.

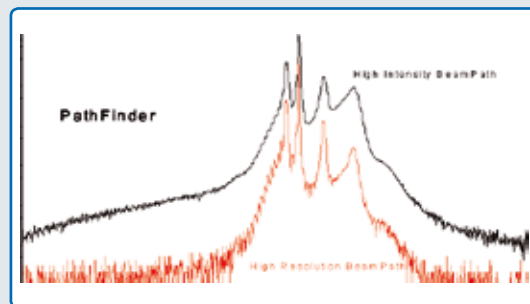


Fig. 3b: Measurement results recorded on the 004 reflection of a three layer $\text{Ca}_x\text{Cd}_{1-x}\text{Te}$ on $\text{Cd}_{1-y}\text{Zn}_y\text{Te}$ substrate; Cu-radiation, high-resolution Göbel Mirror, Germanium (022) 4-bounce monochromator, $\frac{1}{4}$ -circle Eulerian cradle, Pathfinder, and scintillation counter. The black curve represents the result obtained by using the slit, the red curve the results obtained by using the triple-bounce beam path.



Fig. 4a: Phase ID Mirror beam path - XRPD on irregularly shaped sample.

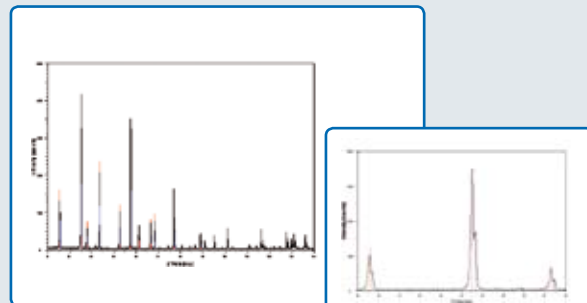


Fig. 4b: Measurement result recorded on NIST 1976 Corundum sample in reflection geometry; Cu-radiation, Phase ID Göbel Mirror, 5° axial Soller slit, rotation sample stage, 0.12° diffracted beam Soller slit, and scintillation counter. The red and blue sticks indicate the peak positions taken from ICDD pattern 46-1212 ($\text{Cu-K}\alpha_1$ and $\text{Cu-K}\alpha_2$). The insert shows the zoomed area from 52° to 62° 2theta; $\text{K}\alpha_1$ and $\text{K}\alpha_2$ separated and the doublet at about 58.8° above the scattering background.

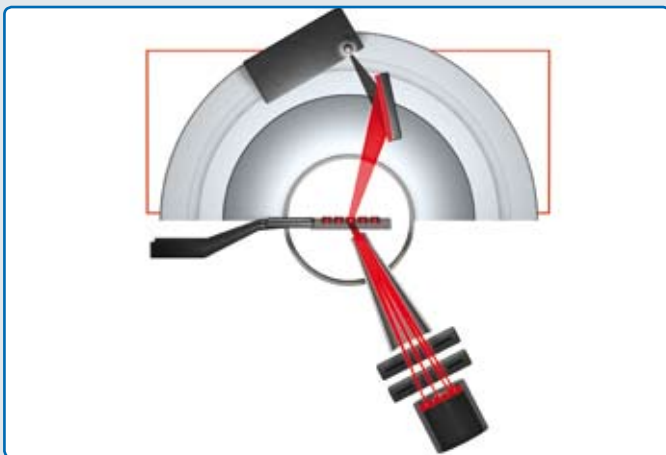


Fig. 5a: Focusing Göbel Mirror beam path – high-throughput XRD in a combinatorial library, in combination with a LynxEye linear detector.

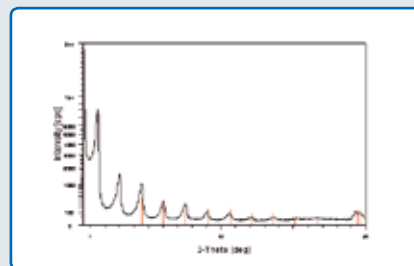


Fig. 5b: Measurement result recorded on silver behenate from 0.5° to 20° 2theta in transmission geometry; Cu-radiation, focusing Göbel Mirror, 5° axial Soller slit, line focus well plate, 8 mm anti-scatter slit opening and LynxEye detector. The red sticks indicate the peak positions taken from ICDD pattern ICDD 4-0048. Remark: the intensities are given on a square root scale.

The different types of Göbel Mirror are available for the most commonly used characteristic emission lines of Cr-, Co-, Cu- or Mo-tubes. Table 2 gives an overview of their most common applications. Actually, numerous applications can benefit from the beam conditioning characteristics of Göbel Mirrors.

Table 2. Recommended applications for the different types of Göbel Mirror.

Göbel Mirror type	Powder sample	Large or complex samples	Reflection and transmission	Thin film	Foil and capillary transmission
Multipurpose	✓	✓	✓	✓	
High-resolution			✓	✓	
Phase ID	✓	✓	✓		
Focusing					✓

Applications which benefit from Göbel Mirrors:

- XRPD on irregularly shaped samples
- XRPD on samples with low absorption
- Kinetic XRPD measurements, e.g. variable temperature, pressure, humidity where sample surface might change
- Residual stress or texture investigations on irregularly shaped samples
- XRPD investigations in transmission and reflection on the same sample, or in the same batch
- Capillary, foil transmission, or high-throughput investigations
- XRR, GID or IP-GID on thin film
- HRXRD of thin films
- μ -XRD on small samples or with μm local resolution

All configurations and specifications are subject to change without notice. Order No. DOC-S88-EXS030 V2.
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