

● **D8 DISCOVER with PILATUS3 R 100K-A** 2D HPC Technology for Your Lab Instrument

Bruker has pioneered 2D diffraction solutions for the lab for more than 30 years. Recently, advances in 2D detector technology at synchrotron beamlines have boosted the interest in 2D diffraction applications tremendously. Bruker's innovative D8 platform and vast 2D application knowledge, combined with DECTRIS' latest Hybrid Photon Counting (HPC) detector technology, results in a powerful diffraction solution for materials characterization. The seamless integration of the PILATUS3 R 100K-A detector into the D8 platform extends the lab measurement capabilities even further.

D8 DISCOVER with PILATUS3 R 100K-A offers:

- Full detector integration into the D8 hardware and software platform
- Continuously variable sample-to-detector distance to balance coverage and resolution
- Gamma-optimized mode to maximize crystallite statistics
- 2Theta-optimized mode to maximize coverage and resolution

Detector Technology

DECTRIS has set the standard for detector technology at synchrotron beamlines across the world in recent years. By combining their latest innovation, the PILATUS3 R 100K-A, with Bruker's expertise in lab based diffraction platforms; a good thing has gotten even better. The PILATUS3 R 100K-A builds on DECTRIS' industry leading HPC technology, including:

- **Instant retrigger**

By instantly reading out and resetting a pixel when its bit depth has been reached, digital saturation effects are a thing of the past, and high count rates can be achieved.

- **Independent pixel response**

When a photon strikes a pixel, only that pixel will respond, which results in an almost ideal point spread function of a single pixel, perfectly matched for measurements with small beam sizes and short sample-to-detector distances.

- **Support of a wide range of incident radiation**

The correct wavelength ensures optimal physical and diffraction space sampling.

- **Air-cooled and maintenance-free operation**

With an air-cooled design and no maintenance requirements, the PILATUS3 R 100K-A is a true asset with low cost of ownership.

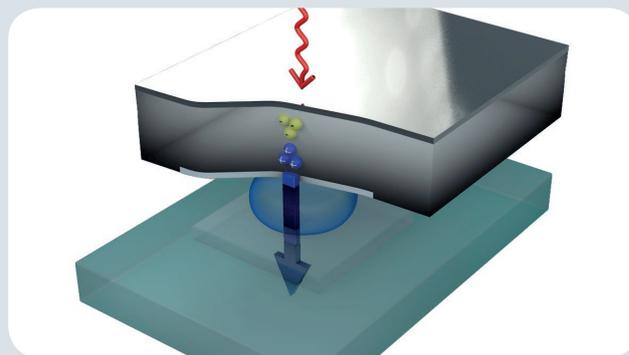


PILATUS3 R 100K-A detector in Gamma-optimized mode

Detector Quantum Efficiency			
Co	1.79 Å	6.9 keV	96 %
Cu	1.54 Å	8.0 keV	98 %
Mo	0.71 Å	17.5 keV	47 %
Ag	0.56 Å	22.2 keV	25 %

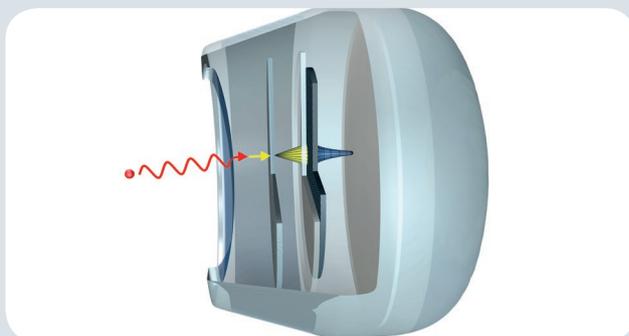
- **HPC Technology – PILATUS3 R 100K-A**

Silicon x-ray detector technology is based on the direct conversion of photons to electrons via the photoelectric effect. Due to the direct nature of this conversion, the position of the photon interaction is accurately measured, which results in an ideal point spread function. The fast conversion also allows for highest count rates and dynamic range.



- **MIKROGAP Technology – VANTEC-500**

MIKROGAP technology utilizes the interaction of x-ray photons with a gas media to create an electron cascade which is collected on a solid anode coated with a limited conductivity material resulting in position sensitive photon counting detection. The technology is easily scaled to large sizes, resulting in the creation of large area detectors while maintaining high quality photon detection characteristics.



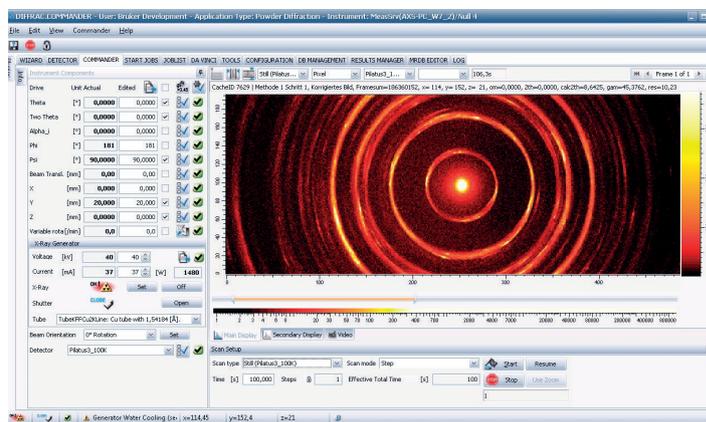
Seamless Integration

The DAVINCI design of the D8 supports upgrades and extensions. This keeps the door open for future applications and performance enhancements. Furthermore, the unique ability to fine-tune the measurement conditions without the need for realignment of the instrument yields the best analysis results.

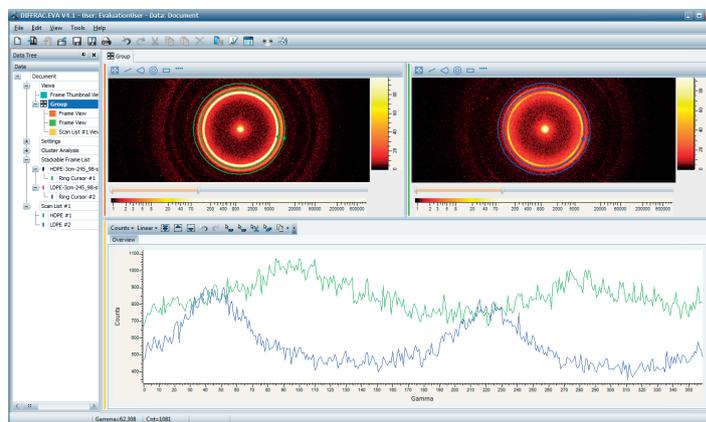
Integrating the PILATUS3 R 100K-A does not stop with having the data streamed to the measurement software. It has been fully integrated into DIFFRAC.SUITE, from immediate measurements in DIFFRAC.COMMANDER, to complex measurement jobs in DIFFRAC.WIZARD and analysis in DIFFRAC.EVA, DIFFRAC.TEXTURE, DIFFRAC.SAXS or DIFFRAC.LEPTOS. These programs not only allow the user to condense the data into conventional intensity versus 2Theta plots, but also to work with the 2D data in its native format, ensuring that the full image can be utilized for advanced analysis.

The PILATUS3 R 100K-A perfectly complements Bruker's state-of-the-art detector portfolio, including:

- LYNXEYE XE-T for 0D/1D/2D diffraction with unmatched energy resolution
- VÅNTEC-500 for instant 2D diffraction with lowest background and largest 2Theta and Gamma coverage



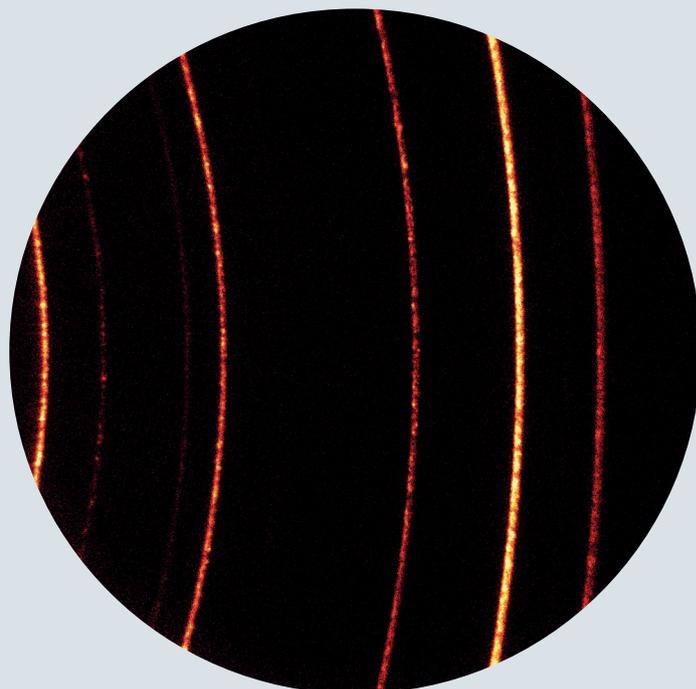
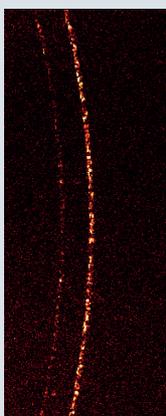
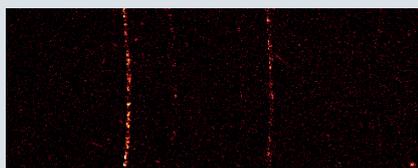
Data collection with DIFFRAC.COMMANDER



Data analysis with DIFFRAC.EVA

PILATUS3 R 100K-A

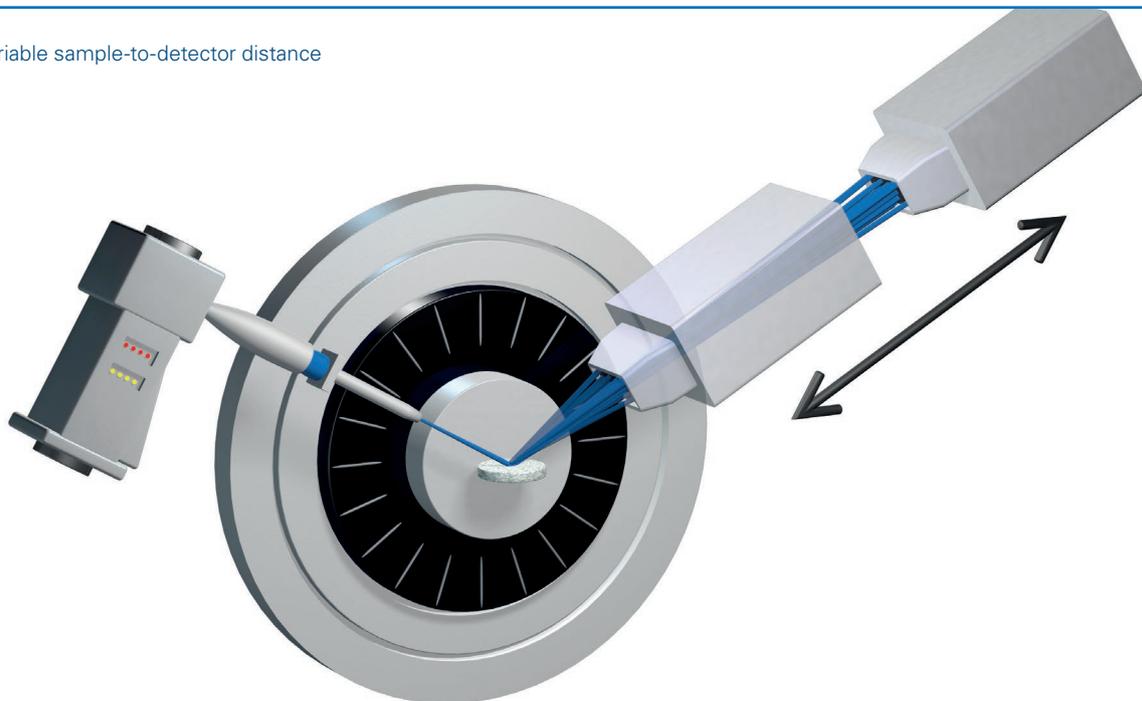
VÅNTEC-500



NIST 1976 (corundum) data collected at sample-to-detector distance of 20 cm.

Left: PILATUS3 R 100K-A (2Theta-optimized Mode)
Middle: PILATUS3 R 100K-A (Gamma-optimized Mode)
Right: VÅNTEC-500

Variable sample-to-detector distance



Balancing Coverage and Resolution

One of the most important instrument parameters to optimize with a 2D detector is the sample-to-detector distance. At a short distance the active area of the detector covers a wide 2Theta and Gamma angular range in a single shot. This may result in very short measurement times, which is beneficial for kinetic studies.

As the detector is moved further away from the sample, a smaller angular range is covered. Angular resolution is improved as each individual pixel element collects a smaller solid angle. Although longer measurement time may be required, the improved resolution helps separate overlapping reflections, which improves phase identification.

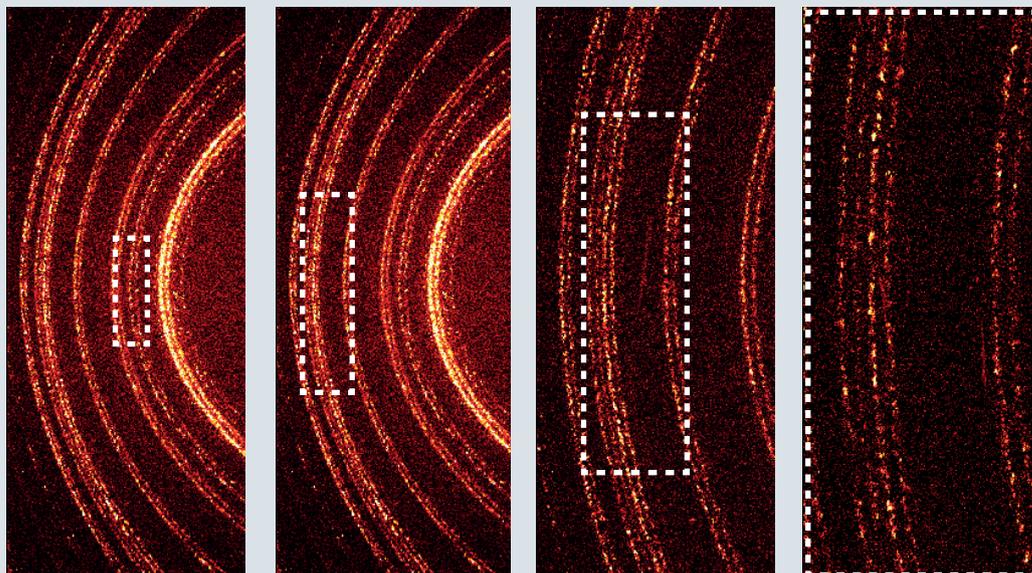
An equally important parameter defining the achievable angular resolution is the incident beam size, which is typically on the order of a few hundred microns for a laboratory instrument. This beam size directly defines the minimum width of a reflection in both 2Theta and Gamma as the beam is projected onto the detector by diffraction.

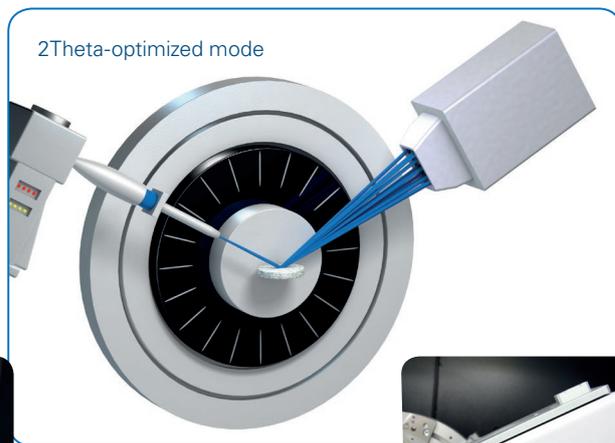
Having the ability to strike the perfect balance between coverage and resolution is an important feature of lab based diffractometers. Ideally this should always be optimized to achieve best data. With the D8 DISCOVER this optimization is trivial and straightforward. In particular the sample-to-detector distance is actively measured in real time, allowing the user to freely set the detector at any position, and the software will automatically load the appropriate calibrations.

NIST 1976 (corundum) collected with sample-to-detector distance of

- (a) 3 cm
- (b) 5 cm
- (c) 10 cm
- (d) 20 cm

The white rectangle represents the 2Theta and Gamma coverage of the PILATUS3 R 100K-A at 20 cm





2Theta versus Gamma Coverage

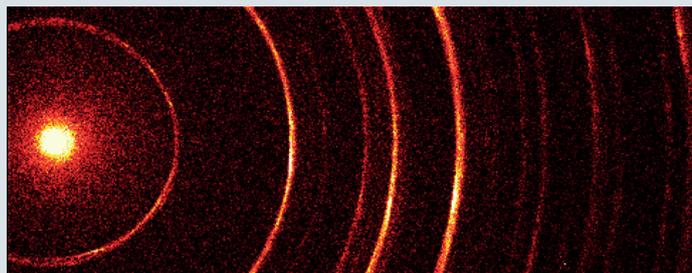
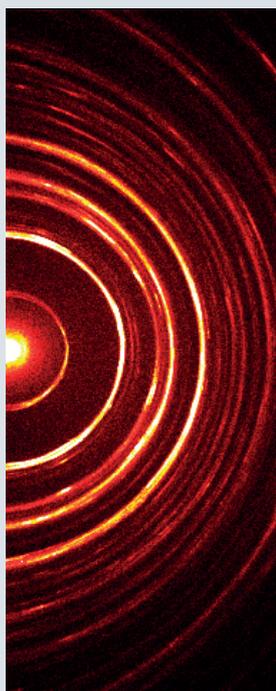
One of the keys to the use of two-dimensional diffraction is the information provided by 2Theta and Gamma. 2Theta is directly linked to probing the inter-atomic spacing (d-spacing) of a sample, while Gamma provides information about the morphology of the sample such as crystallite size or texture.

Thanks to the alignment-free mounting system, the orientation of the PILATUS3 R 100K-A can be quickly set to 0 degrees to allow a large Gamma coverage, or to 90 degrees to achieve a large 2Theta range in a single exposure. Increased 2Theta coverage can be achieved

by repositioning the detector with the high accuracy goniometer.

In Gamma-optimized mode (0 degree), the largest coverage of the diffracted rings is achieved, reducing the effects of preferred orientation and grain size when the data is reduced to a 1D pattern.

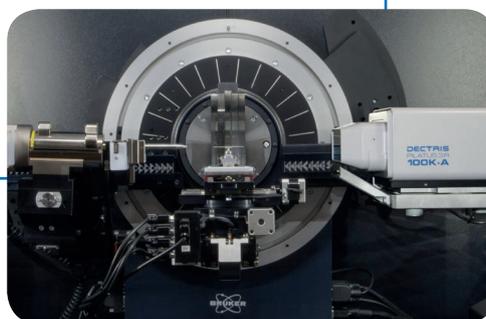
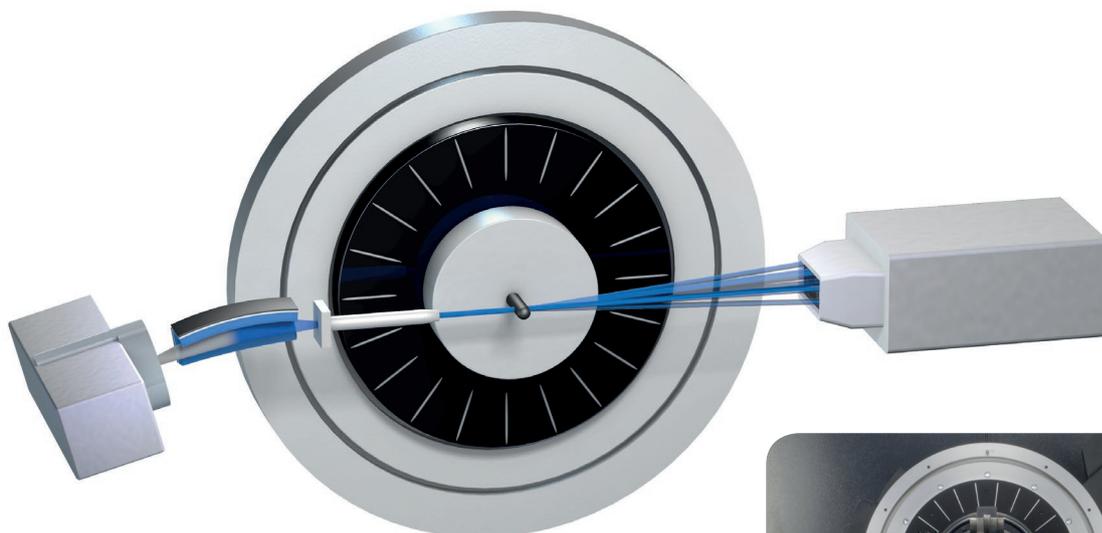
When rotating the detector by 90 degrees, a maximum coverage in the 2Theta direction in a single exposure is achieved, which is beneficial for time sensitive studies. Rotation of the detector can be performed at any time by the user without the need for alignment. Due to real-time component recognition, the software will automatically identify and adapt to the change.



Aspirin tablet measured in transmission with Cu radiation and the PILATUS3 R 100K-A

Left: Gamma-optimized mode with 5 cm sample-to-detector distance
Right: 2Theta-optimized mode with 10 cm sample-to-detector distance

Low angle setup

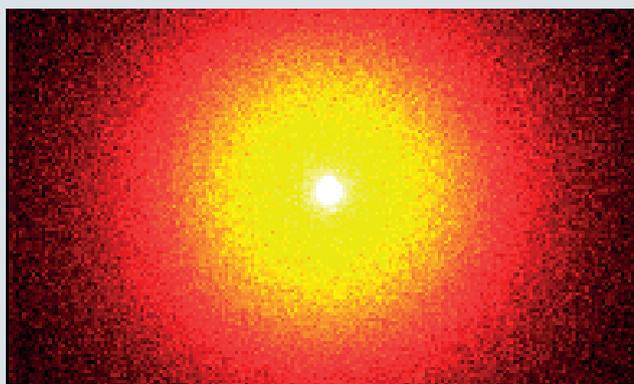
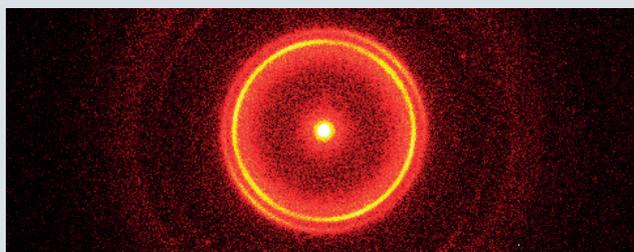


An Unblocked View of Low Angle

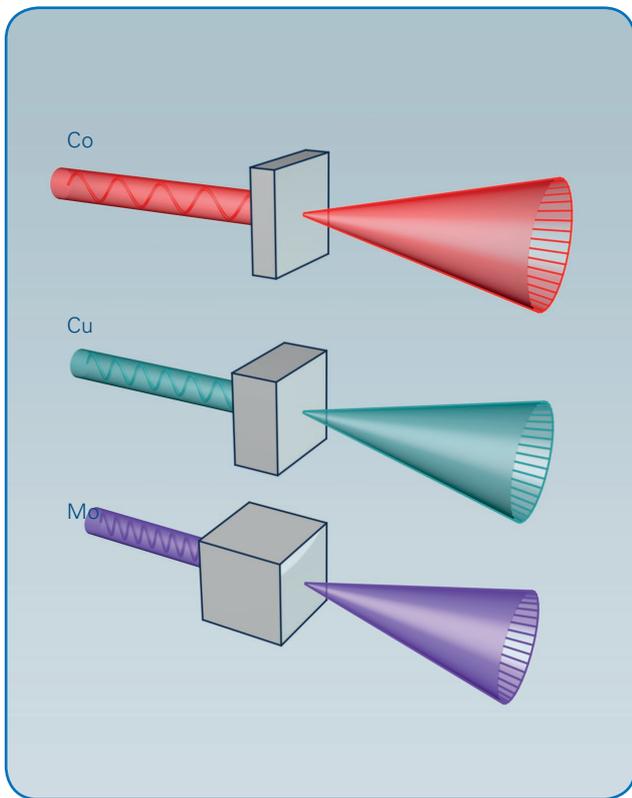
Low angle diffraction measurements have become an important tool for materials research as many samples have length scales in the nanometer range. If the sample exhibits long range order in this length scale, sharp interferometric diffraction effects can be observed, which is common in large molecule and polymer studies.

On the other hand if small crystallites agglomerate into larger particles or large particles decompose into smaller particles, electron density differences between the particles and matrix result in a broadly defined scattering effect.

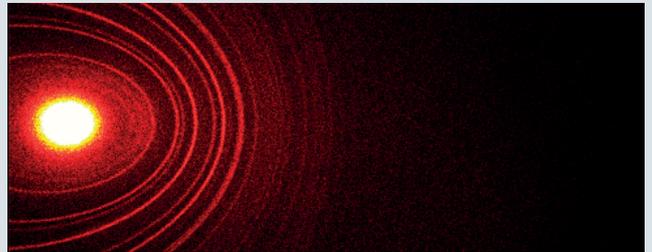
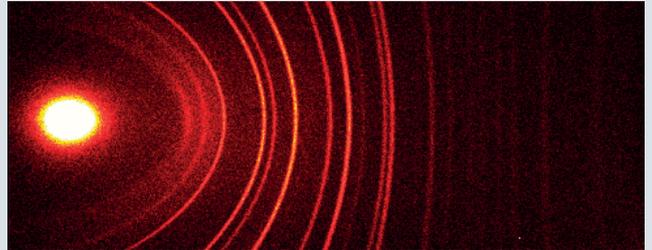
One of the most challenging aspects of these studies has been the clear separation of the direct beam from low angle sample scattering. Even if the detector can withstand the direct beam without damage, a beamstop is typically required to avoid saturation effects which affect the rest of the detector. The single pixel isolation and exceptionally high linear count rate of the PILATUS3 R 100K-A frequently eliminates the need for a beamstop in a lab diffractometer.



Various samples measured in transmission without beamstop:
Top: LD Polyethylene with 3 cm sample-to-detector distance
Bottom: Glassy Carbon with 20 cm sample-to-detector distance



Corundum collected with various radiations and a 3 cm sample-to-detector distance
 Top: Copper radiation
 Bottom: Molybdenum radiation

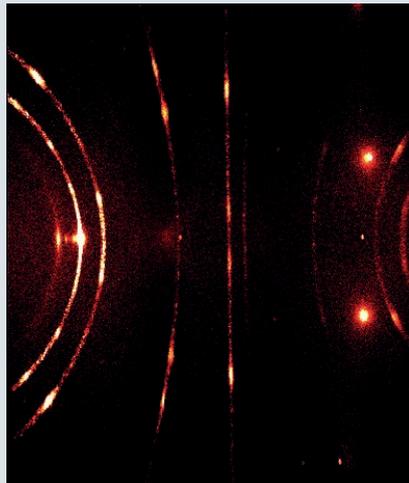
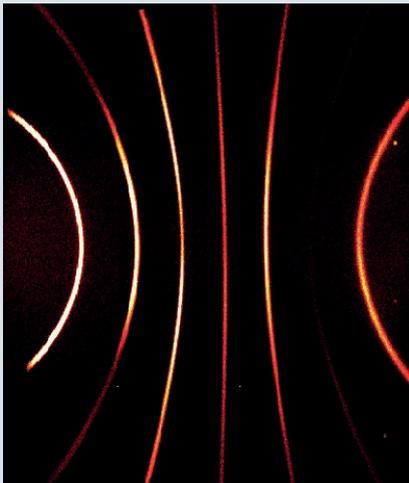


Taking Advantage of the Whole Spectrum

The majority of lab x-ray diffraction systems utilize copper radiation due to its optimal balance of d-spacing coverage and resolution. However, it may be advantageous to use other characteristic radiation energies. For steel samples, cobalt is used to reduce sample fluorescence and to shift favorable intensity reflections to high angle for better strain sensitivity. If deeper penetration or transmission geometry is required, a higher energy such

as molybdenum radiation may be required. This higher energy radiation also gives access to a wider range of d-spacings and consequently is a better choice for applications such as PDF analysis. The PILATUS3 R 100K-A is compatible with a wide range of characteristic wavelengths. The ability to change a conventional sealed x-ray tube can be accomplished in a matter of minutes by a standard user.

Textured Thin Film Diffraction



Textured thin films on silicon wafers measured at 3 cm sample-to-detector distance:

Left: Tungsten film showing weak texture

Center: Copper thin film showing strong texture

D8 DISCOVER with PILATUS3 R 100K-A for Advanced Materials Research



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