

## CHEMICAL CRYSTALLOGRAPHY

# D8 VENTURE HE

Cutting-Edge Solution for  
High-Energy Crystallography

Innovation with Integrity

# D8 VENTURE HE – Your dedicated solution for high-energy crystallography

## The unique benefits of high-energy crystallography

High-energy crystallography in the home lab is typically performed using Mo or Ag X-ray sources. Since X-ray absorption scales with wavelength, higher energy radiation can greatly improve the quality of data from inorganic and mineral samples, as lower absorption and reduced extinction reduce the reliance on data correction.

Ag radiation provides more compressed reciprocal space, which offers huge benefits:

- More complete data can be collected in geometrically restricted experimental setups, such as when using DACs for high-pressure studies. Data collection in diamond anvil cells (DACs) also benefits from the very small beam generated by the  $\mu\text{S}$  DIAMOND II to minimize diffraction from the diamond anvils and from the gaskets.
- Charge density studies also benefit from the compressed reciprocal space that Ag radiation provides. The diffraction geometry of the D8 VENTURE HE allows data to be reliably collected with the highest accuracy to  $0.33 \text{ \AA} / 1.5 \text{ \AA}^{-1}$  in short measurement times.
- Access to higher resolution offers the possibility for the analysis of pair distribution functions (PDF analysis).

Previously, the benefits to crystallography of using higher energy radiation have been offset by the relatively weak high-energy X-ray sources and detectors optimized for work at lower energies in the Cu to Mo range. These restrictions led to unacceptably long measurement times and lower quality data.

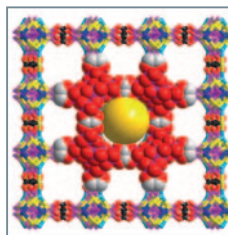
## D8 VENTURE HE – the power to perform

As a new addition to the D8 VENTURE family, the D8 VENTURE HE combines, for the first time, the unique high intensity of the  $\mu\text{S}$  DIAMOND II, with the PHOTON III HE photon-counting, detector optimized to achieve the highest quantum efficiencies for Mo and Ag radiation, for single and dual wavelength solutions.

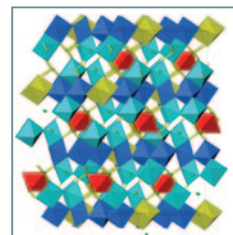
With the versatility of a Mo source, the D8 VENTURE HE is a highly productive instrument for the service crystallography facility and delivers the best data for inorganic, solid-state, and geo-chemists. The short-wavelength Ag source provides access to the most demanding experiments for physical chemists.

## D8 VENTURE HE – in short, the most useful system for the solid-state chemistry laboratory

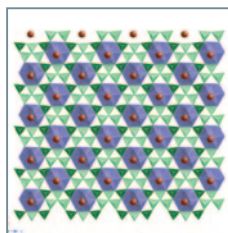
Service  
crystallography



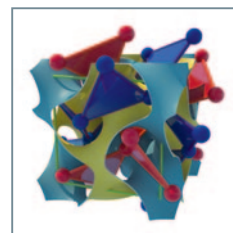
Minerals



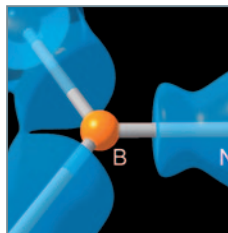
Strong absorbers



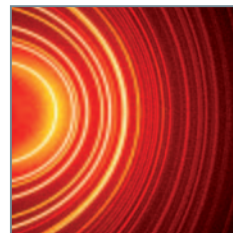
Inorganic



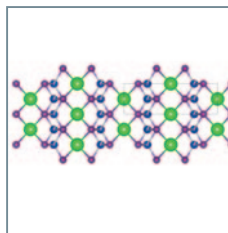
Charge density



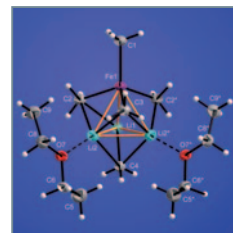
Powder



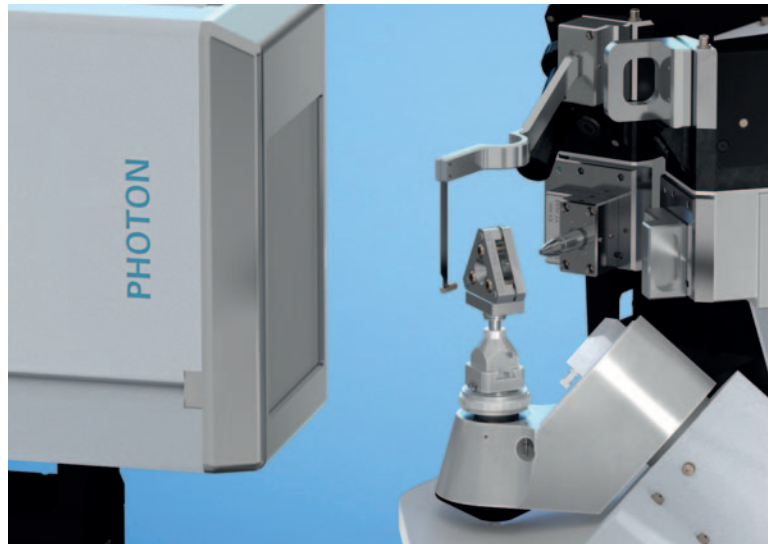
High pressure



Coordination

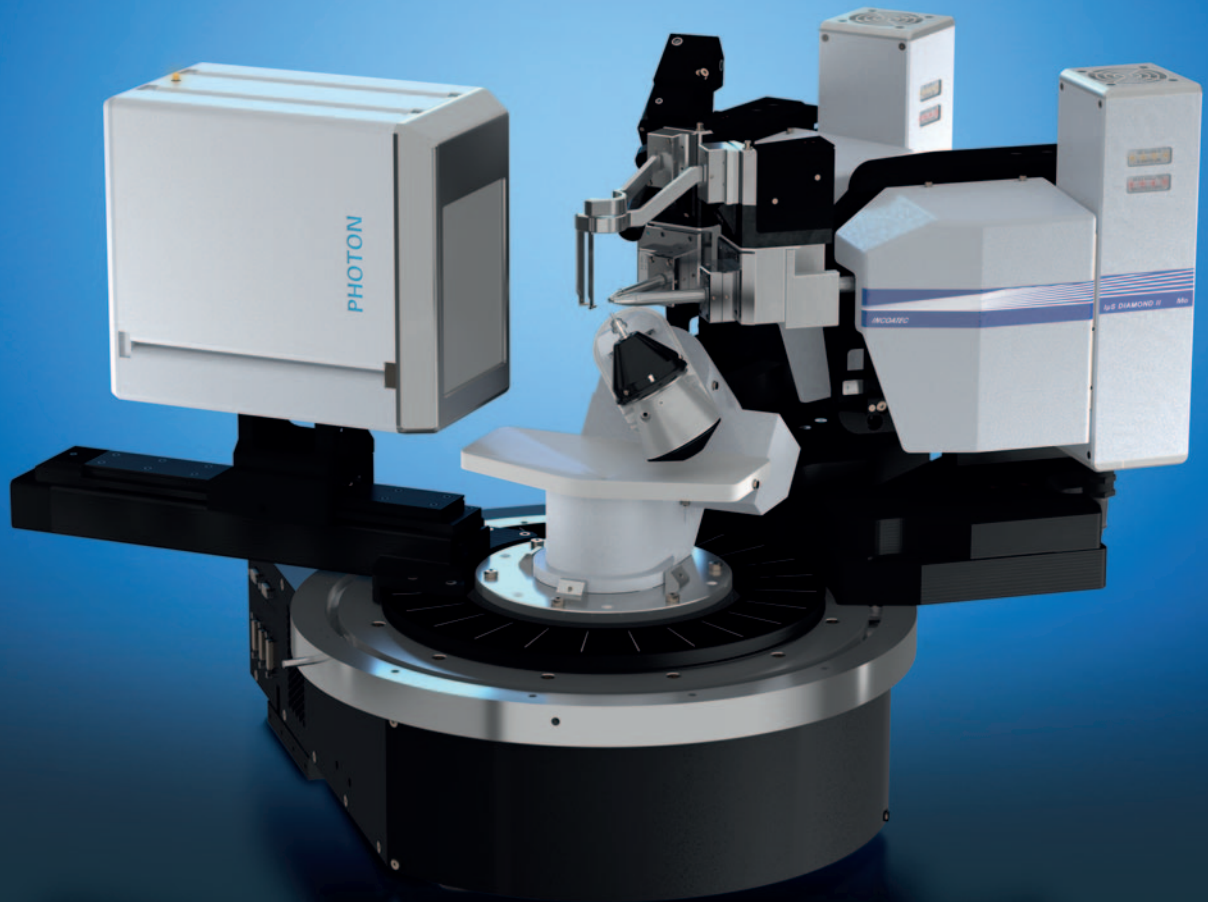


The High-Pressure Kit accommodates most commercially available diamond anvil cells. It is safe and easy to switch between standard and high-pressure setups in only minutes.



## D8 VENTURE HE

- Configuration example:
- I $\mu$ S DIAMOND II, Mo
  - I $\mu$ S DIAMOND II, Ag
  - HELIOS optics
  - KAPPA goniometer
  - PHOTON III HE detector



# 1 $\mu$ S DIAMOND II – highest intensity, proven reliability

The highest intensities are achieved in the 1 $\mu$ S DIAMOND II by optimizing all the critical tube parts, such as the cathode, electron optics and take-off angles.

The diamond hybrid anode used in the 1 $\mu$ S DIAMOND II features an isotopically pure diamond substrate that is coated with a layer of the target material for vastly improved heat management. A high-brightness cathode with active electron lens provides the most homogeneous electron beam and allows fast ramp-up and ramp-down.

Combined, these innovations mean the 1 $\mu$ S DIAMOND II delivers X-ray intensities an order of magnitude greater than conventional microfocus sealed tubes, and that outperforms conventional microfocus rotating anodes.

## Get more from your instrument

Shorter measurement times and reliable, instantaneous wavelength switching makes dual-wavelength data collections a reality and opens the door to a world of new opportunities for your research.

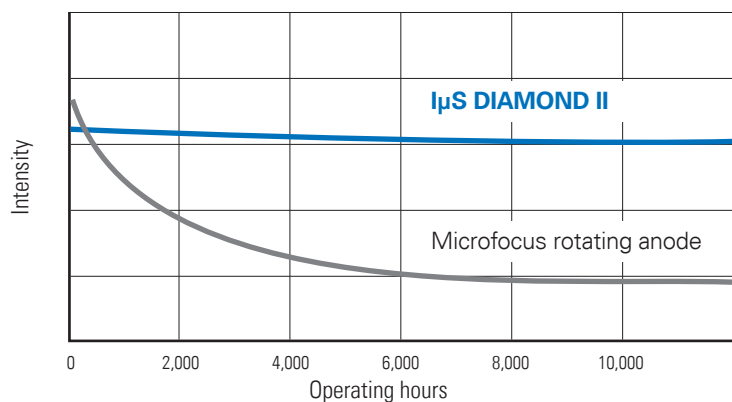
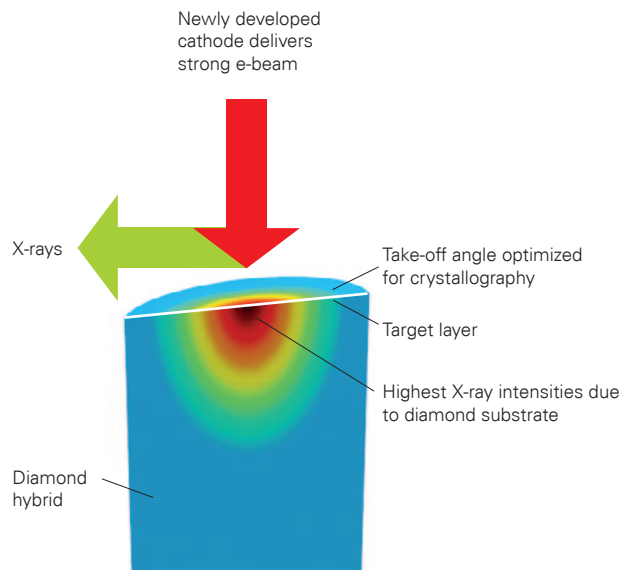
## Rotating anode performance with sealed-tube convenience

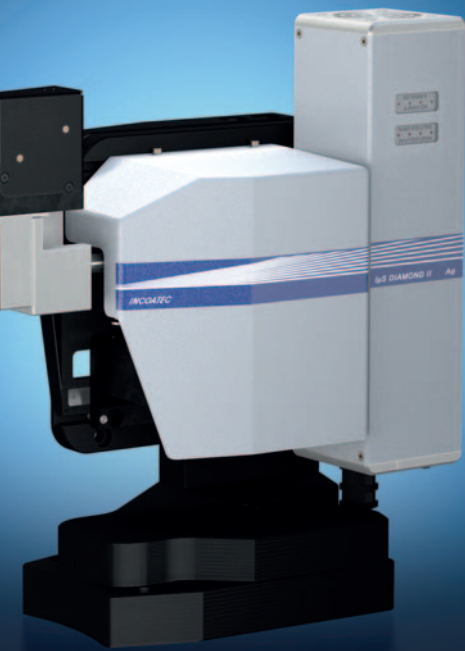
Rotating anodes suffer rapid degradation of output due to repeated heating-cooling cycles of the anodes, leading to micro fractures at the surface. In contrast, the heatload on the 1 $\mu$ S DIAMOND II target is constant over time, making the output ultimately stable. Even better, the 1 $\mu$ S DIAMOND II outperforms microfocus rotating anodes without the high running costs and the headache of regular maintenance.

Fully air cooled, no moving parts and optimized heatload management means the 1 $\mu$ S DIAMOND II has very long tube lifetimes and requires no routine maintenance in-between.



## 1 $\mu$ S DIAMOND II hybrid anode, Mo and Ag





# PHOTON III HE: large area, photon-counting detectors optimized for high-energy

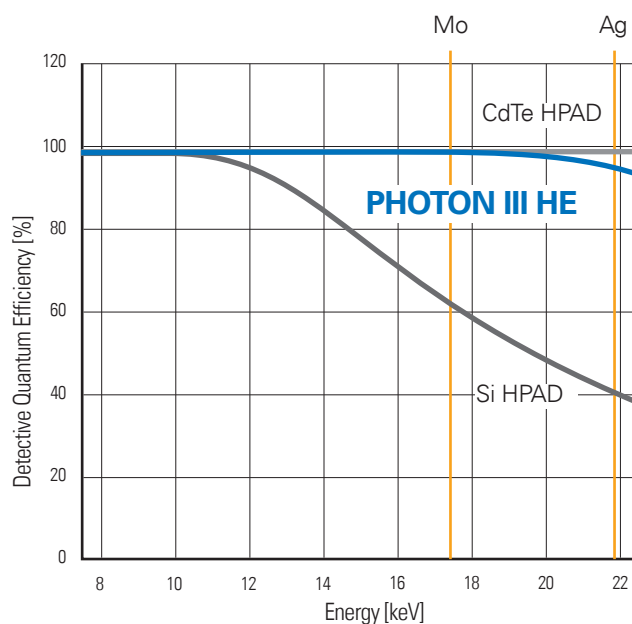
The PHOTON III HE achieves comparable Detectable Quantum Efficiency (DQE) to CdTe HPADs with Ag and Mo radiation and offers a much larger active area. In total the PHOTON III HE delivers the best data in the shortest time.

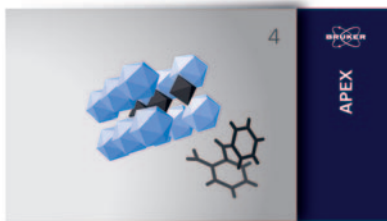
The PHOTON III HE uses a new rare-earth X-ray converter that achieves near-ideal Detectable Quantum Efficiency (DQE) for X-rays in the 15 to 25 keV energy range. This makes the PHOTON III HE the ideal detector for use with Mo and Ag X-ray sources.

PHOTON III HE is built on the same design as the successful PHOTON III detectors and uses the proven technique for photon counting based on charge integration.

The PHOTON III HE detectors employ large monolithic sensors with no insensitive regions. This allows you to collect highly accurate data very efficiently to very high resolution, when your experiments require larger sample-to-detector distances or when higher data multiplicity is required to get the very highest accuracy, for example in charge density measurements.

## Absorption efficiency of X-rays

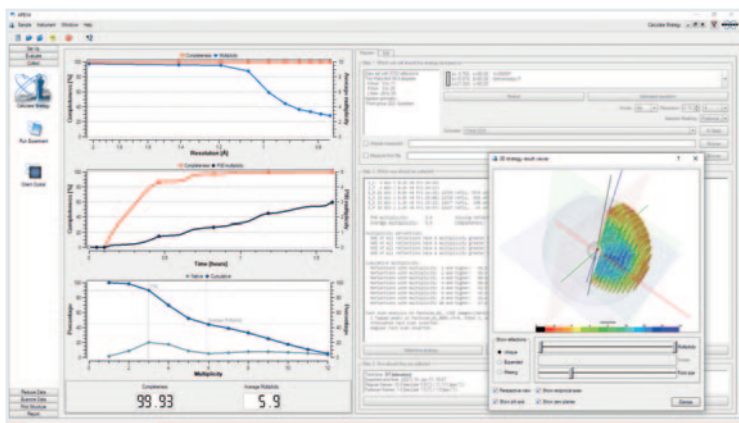




## Data Collection Strategy Planning

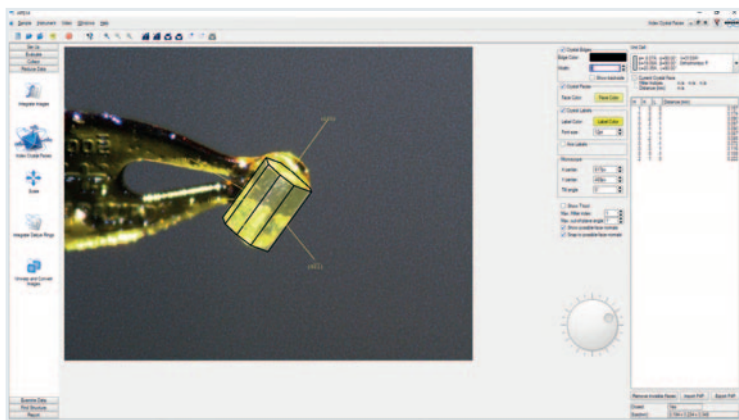
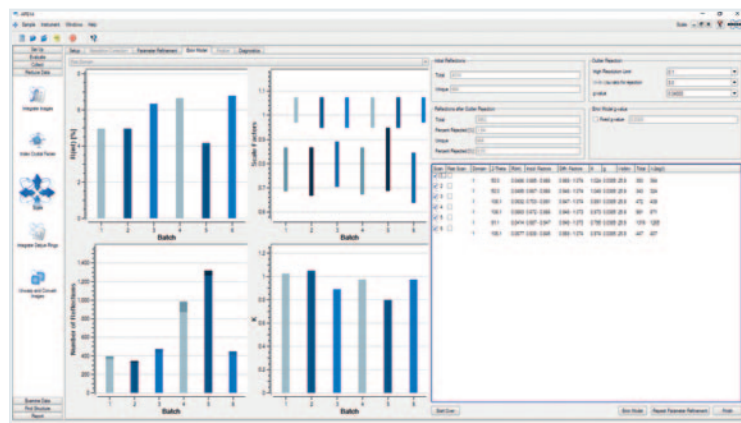
Make the most of your instrument time and collect complete data fast and efficiently. The APEX4 suite ensures highest possible completeness and optimized instrument usage.

Confidently rely on an automated strategy determination that lets you adjust parameters as you are always in the driver's seat.



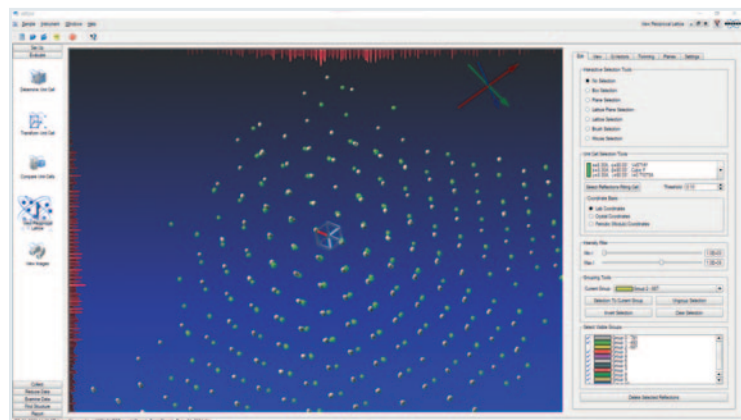
## Scaling and Absorption Correction

Solid state compounds can exhibit strong absorption even with high-energy radiation, and high-pressure experiments can pose their own challenges. Good empirical absorption correction and scaling are paramount for the best data.



## Face Indexing

APEX4 easily and intuitively describes a crystal's shape from a pre-recorded movie with easy-to-use tools and intelligent helpers. Combined with higher-energy radiation gives the best data from the most strongly absorbing samples.



## Reciprocal Lattice Viewer

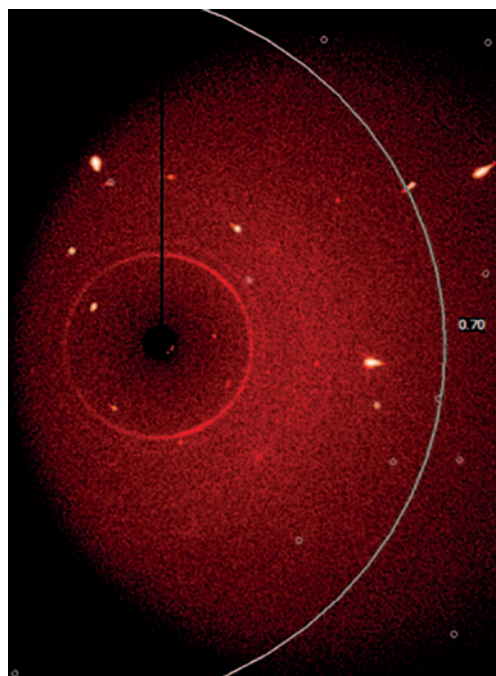
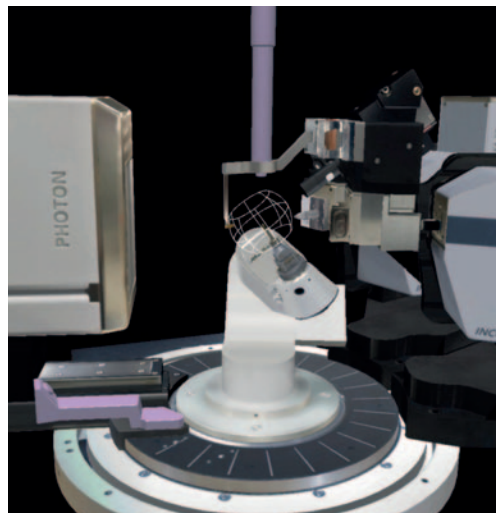
Our GPU-accelerated plug-in enables you to easily handle challenging samples interactively to modifying reflection arrays. Visually separating multiple lattice components is now faster than ever. The many new options make APEX4 the most powerful tool for advanced crystallography.

# APEX4 – all the tools for the most demanding experiments

## Getting the best results from diamond anvil cells

- Component recognition for path planning and collision avoidance
- Powder ring exclusion during reflection harvesting
- Powerful indexing methods to identify orientation matrices of the sample and the diamond anvil crystals
- Concurrent handling of multiple matrices during data integration
- Concurrent handling of multiple Bravais lattices during data integration
- Dynamic image mask for modeling the partial shading of the diffraction images by the DAC
- Proven “best-plane” background treatment of inhomogeneous and rapidly changing backgrounds
- Comprehensive interface for analyzing the integrated data and outlier detection

System ready for mounting the diamond anvil cell, as visualized in the path planning software. Active path planning makes hardware collisions impossible.



Diffraction image from a single crystal in a diamond anvil cell recorded on a PHOTON III HE detector. The image shows strong reflections from the diamond anvil crystals, weaker reflections from the sample crystal. Also present are the DAC shadow and high background scatter, both of which typically change rapidly from frame to frame.

## Overview of Features and Benefits

### Main characteristics

<b>D8 VENTURE HE</b> System	The D8 VENTURE HE is the first system for dedicated solid state chemistry research. It combines the unique high intensity of the $\mu$ S DIAMOND II with the PHOTON III HE photon-counting detector.
	The D8 VENTURE HE is available in single and dual wavelengths configurations with Mo and Ag X-ray sources.
	Our robust sample stage handles weights up to 2 kg while retaining the specified sphere of confusion (SOC). Custom-made solutions for heavier and bulky cells are available on request if your research is demanding even more.
	APEX4 includes all the tools needed to successfully treat the challenges in solid state crystallography.

	Feature		Benefit
<b>PHOTON III HE</b> Detector	Photon-counting pixel-array detector	5th generation pixel-array detector technology	Higher speed and sensitivity, best data quality
	Large active area	100 × 70 mm <sup>2</sup> 100 × 140 mm <sup>2</sup>	Faster data collection
	Fast readout time	14 msec	
	Very high count rate	Up to 4 × 10 <sup>6</sup> counts/pixel-sec	
	Readout dead time	0 sec (full shutterless operation)	
	No dead areas	Single, monolithic silicon sensor	Improved data quality
	No charge-sharing noise	0 electrons charge-sharing noise	
	Very low parallax	< 1 pixel	
	No count-rate nonlinearity	< 1 % nonlinearity up to full count rate	
	High detective quantum efficiency (DQE)	Mo 99 %, Ag 95 %	No maintenance, high uptime
No operating gas or cooling water	Completely sealed design, air cooled		
High reliability	Warrantied for 3 years		
<b><math>\mu</math>S DIAMOND II</b> Source	Very high intensity beam, completely air cooled, revolutionary e-beam and cooling technology	Mo and Ag radiation	Dual-wavelength configuration with instantaneous wavelength switch for advanced data collection. Shorter measurement times and better data from difficult samples.
<b>D8</b> Goniometer	Very low sphere of confusion	< 7 $\mu$ m	Best data quality
	High speed	Up to 1,200 deg/min (omega)	Faster data collection
	Kappa geometry		Highest flexibility
<b>APEX4</b> Software	Most comprehensive software package for single crystal X-ray diffraction (SC-XRD) using well-tested first-class algorithms		
	User-selectable level of automation: for novices and/or complete control for experienced crystallographers		
	State-of-the-art responsiveness: incorporating user feedback from hundreds of installations		
	Unparalleled twin handling: the most powerful reciprocal lattice viewer to tackle all crystallographic problems		
Model Building: first-class interactive model-building and refinement powered by SHELXLE			

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