APEX II QUAZAR with Ag radiation – Unparalleled microfocus performance for solid state chemistry

As a new addition to the APEX II QUAZAR family the world's first microfocus source for Ag radiation is now available. For the first time it is possible to operate a high intensity Ag source with less maintenance than a standard sealed tube and without the hassle of a rotating anode. Like the other versions of the IμS the source is built from the finest components, extremely powerful and reliable.

The APEX II QUAZAR is the system of choice for inorganic solid state compounds.

Silver radiation can greatly improve the quality of data from inorganic and mineral samples as lower absorption and smaller extinction decrease the need for data correction. Charge density studies benefit from the "compressed" reciprocal space that Ag radiation provides. Diffraction geometry allows data to be reliably collected to a resolution of 0.33 Å / 1.5 $Å^{-1}$.

Shorter wavelength also improves data collected on very strong absorbers. The very small beam sizes that are achievable with the Ag microfocus source are ideal for high pressure experiments with diamond anvil cells.

Ag IμS – The world's first Ag sealed tube microfocus source

The Ag IμS is a superb combination of our Ag microfocus source and QUAZAR optics especially designed for Ag radiation. Once again Bruker is setting a milestone by designing and manufacturing highly efficient multilayer optics for shorter wavelengths.

Both source and multilayer optics are carefully matched to each other to provide you with a small, high-intensity beam that is appropriately sized for the small samples seen in today's research.

The intensity of the beam is more than 2 x 10^9 photons/(s mm^2). This generates diffracted intensities of more than 3 times compared to a standard 1.5 kW Ag sealed tube system with a graphite monochro-mator.

Ag IμS with optics

Higher intensities are difficult to achieve even with rotating anodes since the high ductility and low melting point of silver make it a less than ideal target material, with short anode life times and high maintenance. The Ag IμS on the other hand is more reliable and has less maintenance than a standard sealed tube.

Like the Cu and Mo versions the Ag source is operated at only 30W. The Ag tube lasts as long as the well established Cu and Mo tubes that set the standard for modern microfocus sealed tube systems. Water cooling is not required and maintenance and cost of ownership are very low. Despite the low power consumption the X-ray beam has a high brilliance and unprecedented high flux. The Ag tube makes the APEX II QUAZAR the world's first microfocus system operated at Ag wavelength of 0.56 Å.

3-year warranty on the entire source

Bruker's microfocus systems not only deliver the most intense X-ray beams in their class, they do this reliably over long periods of time. The X-ray source including the multilayer optics comes with a full three year warranty. The systems are stable and reliable. This means no downtime due to tube changes or mirror alignment – guaranteed!

QUAZAR optics

The Ag multilayer optics generates a focused beam that provides maximal intensity at the sample.

Significantly improved production methods, including an enhanced control of the deposition process make Montel-type mirrors for Ag radiation available. The optics is protected in an evacuated enclosure. The alignment under vacuum guarantees a stable, high intensity X-ray beam.

Homogeneous Gaussian shaped beam

APEX II – The best detector for solid state chemistry

The APEX II incorporates a full size 62 mm square CCD chip with 4K * 4K (16 mega) pixels. Smaller CCD-chips used in other designs require a fiber optic taper to obtain a comparable active area. Over 90% of the photons from the phosphor screen are lost in the fiber optic taper. The revolutionary APEX II design featuring 1:1 imaging improves the optical transmission by an order of magnitude and minimizes spatial distortion. The excellent spatial resolution and superb point spread function guarantee accurate unit cell parameters for the even most challenging samples.

Cooled to -60° C the APEX II has an impressively low dark noise, which, combined with the fast, low noise readout electronics, provides the high dynamic range of 1:50,000. Electronic dithering prevents overflows of saturated pixels into neighboring regions. This makes it the ideal detector for both strong and weak diffracting samples as well as diffuse scattering experiments where strong reflections need to be recorded next to weak diffuse signals. The detector is optimized to provide best results for a wide range of wavlengths, e.g. Ag, Mo or Cu radiation.

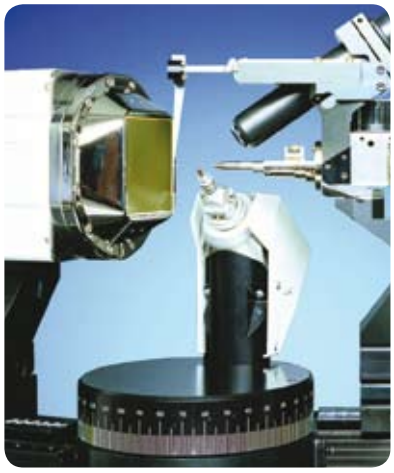
The APEX II is the "gold standard" for chemical crystallography.

Fixed-Chi or KAPPA – smallest sphere of confusion guaranteed

Based on the highly accurate D8 goniometer which maintains superb alignment for many years the APEX II QUAZAR is offered with 3-circle or 4-circle goniometers. D8 mechanics are so precise that the sphere of confusion or error in intersection of the instrument axes is 7 microns or less – far smaller than any other 3- or 4-circle goniometer design. This ensures that even the tiniest microcrystals will remain in the center of the instrument. Reliable collision protection in software and hardware safeguards your investment and allows for efficient and fully automated data collection strategy planning.

Fixed-Chi 3-circle goniometer – simplicity and efficiency

The open geometry allows for complete data sets for any crystal symmetry by using a combination of phi and omega scans. Omega can swing for a full 180° beneath the collimator for highly efficient data collection.



Fixed-chi goniometer

Kappa 4-circle goniometer – goniometer versatility

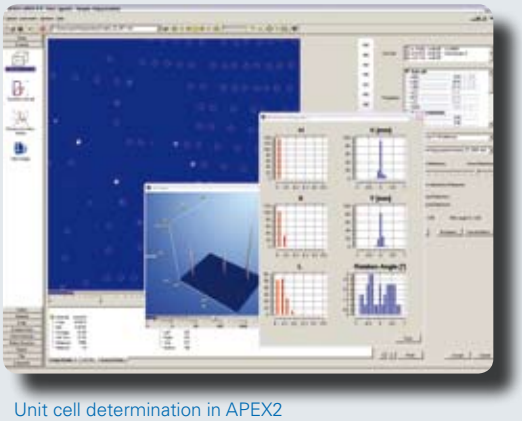
The compact Kappa goniometer offers full sample positioning freedom and a motorized detector track. All axes intersect within a 7 micron sphere.

Kappa goniometer

APEX2 Software – The best software for solid state chemistry

The powerful APEX2 software takes a completely new approach to how you interact with a crystallographic experiment. The Graphical User Interface (GUI) guides you through the complete experiment with minimal user input and maximal graphical feedback. The APEX2 software follows a plugin concept that provides all the individual subroutines and tools needed for structural work. Plugins communicate with each other through a database ensuring the integrity of the determined values at any time. GUI launches required modules with a mouse click. APEX2 is the only software with remote control built in with a true client server architecture that lets you connect to your instrument from virtually anywhere.

APEX2 for solid state chemistry



Unit cell determination in APEX2

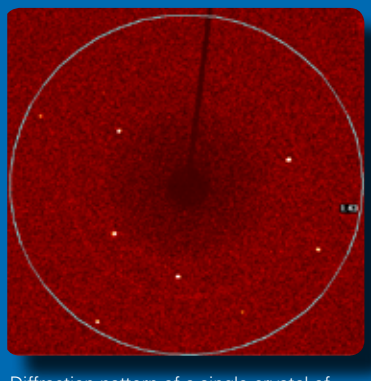
- Calculated precession images
- Diffraction space viewer
- Powder integration
- Simultaneous data integration and scaling of up to eight domains in e.g. a non-merohedral twin
- Modulated and composite structures

"We were investigating a crystal that shows a temperature dependent phase transition that creates a systematically inter-grown six-fold twin. APEX2 was crucial for data processing. Understanding and solving this puzzle with APEX2 convinced me how powerful this package is. I don't believe that any other commercial software is capable of handling these complex problems, at least not as elegantly as APEX2."

Dr. Juergen Nuss, MPI Stuttgart, Germany

APEX II QUAZAR – Applications

High Pressure studies

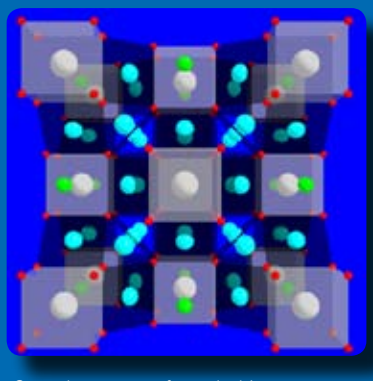


Diffraction pattern of a single crystal of gabapentin heptahydrate ($C_9H_{17}NO_2 \times 7H_20$)

Crystals were grown in-situ in a Be-free DAC and data were collected on the APEX II QUAZAR with Ag-radiation. Diamond reflections from the DAC are significantly smaller and the background is greatly reduced. <I/σ> is increased from18.3 (Mo) to 19.6 (Ag) and more than 20% more unique reflections are accessible.

Dr. Francesca P. A. Fabbiani,
Georg-August-University, Göttingen, Germany

Highly absorbing solid state samples

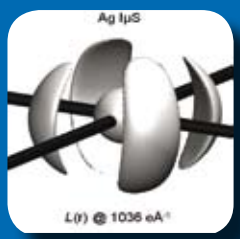


Crystal structure of murdochite ($Cu_6PbO_7(Cl,Br)$)

The shortest wavelength available for an in-house SC-XRD system provides many more reflections within the same 2-Theta range and improves the data to parameter ratio. This allowed the anisotropic refinement of the O and Cu atoms in murdochite. Lower absorption results in a superior signal to noise ratio compared to Mo data. Residual density peaks in the high-resolution Ag data set were obtained from the conventional monopol-refinement model and contain valuable information on the electron distribution within the chemical bond.

Dr. Th. Malcherek,
Hamburg University, Germany

Electron density studies



L (r) in the valence region of the Co atom

Residual Electron Destiny Map (cut at 0.8 $Å^{-1}$, contours at 0.05e$Å^{-3}$ interval)

The Laplacian of the charge density of Sc_3CoC_4 determined from data collected with an APEX II QUAZAR with Ag IμS is very consistent with the theoretical model and reference data quoted in J. Chem. Soc. 2007, 129, 9356-9656.

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