

Upgrade your KAPPA CCD

Take your KAPPA CCD system to the highest level of data quality

KAPPA CCD's have been the first single crystal X-ray diffraction solutions offering the combination of the KAPPA geometry and a CCD X-ray detector. Since 2002 this system is no longer sold, but a large number of its design features have made it into our current instruments:

- Our current KAPPA APEX II combines two magnificent components: the D8 goniometer base, with an unequalled Omega and 2Theta axes precision, and the Original KAPPA stage as it had been designed for the KAPPA CCD. Since the D8 is an extremely precise and reliable goniometer, it is the predominantly used system in materials research. The KAPPA geometry has been invented by Bruker to allow an open access to the sample. As a matter of fact this excellent combination of properties constructs a goniometer, which has a sphere of confusion of just 7 micron, better than any other KAPPA goniometer available in the market.
- The COLLECT software is well accepted by KAPPA CCD users' community. Users in particular appreciate its level of automation, computing sensible default data collection parameters for each sample as much as the seamless integration of data evaluation and structure solution packages. The COLLECT-suite has been a great source for program routines and code for our current APEX2

software package. As in COLLECT most of the routines and procedures use Python programming. Python opens an opportunity for individual modification and for adaptation of the program to special requirements at a user-level.



Figure 1: KAPPA CCD with APEX II CCD detector.

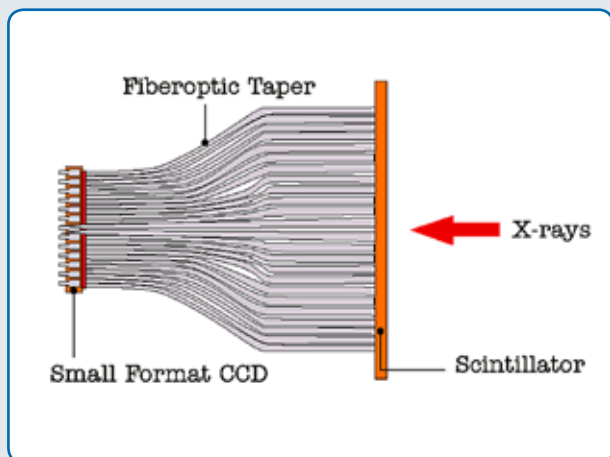


Figure 2: Design of the KAPPA CCD detector (includes fiber optic taper).

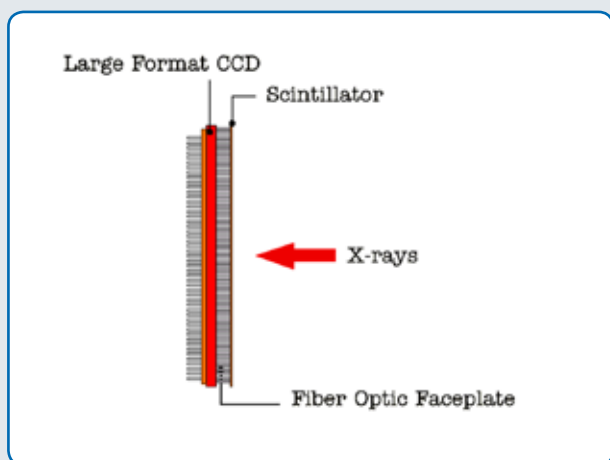


Figure 3: Design of the APEX II detector (no reduction taper)

- High sensitivity
- No spatial distortion
- Low noise
- Wide dynamic range

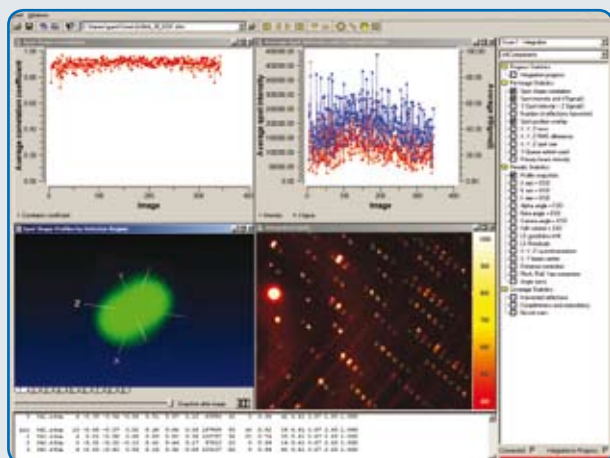


Figure 4: Data Integration.

COLLECT users will discover many features they are familiar with in the latest APEX2 release:

- Phi/Chi scans for a quick unit cell determination.
- Oriented scans which allow to get information on the Laue symmetry prior to a data collection.
- Friedel pairs can be measured in the same image, which avoids incorrect determination of the anomalous signal in case of a decaying crystal.
- Pseudo-precession routines to check for diffuse scattering and modulation.
- Efficient data collection strategy determination procedures.
- Suggestion of suitable data collection time using intensity obtained from frames collected for indexing.
- Suggestion of scan-width, based on the mosaic spread.
- Suggestion of useful crystal-to-detector distance, based on beam divergence, lattice parameters and mosaic spread.
- Determination of the maximal useful resolution (diffraction angle).
- APEX2 stores data collection and processing parameters in a similar way COLLECT does.

On the other hand APEX2 has an number of features, which were less pronounced in COLLECT or not even available at all:

- APEX2 comes with an advanced graphical user interface, which provides a much better graphical feedback to the user than the COLLECT suite ever did. In particular for novice user this greatly facilitates familiarization and the use of the software.
- The RLATT plug-in is greatly appreciated by the installed users' base, since it allows for an excellent visualisation and user interactive investigation of the reciprocal space. In particular this is highly appreciated for analysing twinning and incommensurate or modulated structures.
- APEX2 can handle up to 8 (eight) orientation matrices from inter-grown or twinned crystals. The software simultaneously distinguishes between non-overlapping, partially-overlapping, and fully-overlapping reflections for each of the up-to-eight specimens. Combined with an efficient scaling and absorption correction routine this ensures first-class results even for the "difficult crystals". In fact they are "no-longer-difficult" these days.
- The PHASE-ID plug-in integrates data from your powder

sample and enables for the use of professional powder software package, such as EVA or TOPAS. The quality of data and the user friendliness offered by PHASE-ID clearly outperform those of POWDERIZE.

- The newly developed diffraction space viewer is the ideal tool for the investigation of textured samples, fibers and Non-Bragg diffraction.
- For a fully automated structure solution and data refinement APEX2 comes with the AUTOSTRUCTURE routine. AUTOSTRUCTURE refines the model against a large library of real life examples and is particularly useful for samples from organic and metal-organic chemistry.
- The propriety version of SHELXTL is now fully integrated into the APEX software and available for Windows and Linux. The SHELXTL program suite includes XPREP for space group assignment, statistics, numerical absorption corrections, display of calculated Patterson sections, merohedral detwinning and much more. SADABS handles scaling and multiscan absorption correction. XS, XL and XM form the heart of the structure solution and refinement package. XP and XSHELL provide atomic and molecular graphics, XCIF produces reports from standard CIF files with formats for direct deposition to journals and databases. Cell_now and TWINABS have been added for advanced treatment of twin structures.

The latest COLLECT version allows to write KAPPA CCD images in a format, which is read by the APEX2 software suite. All KAPPA CCD users can take advantage of our new software developments - instantly.



Figure 8: APEX II CCD detector.

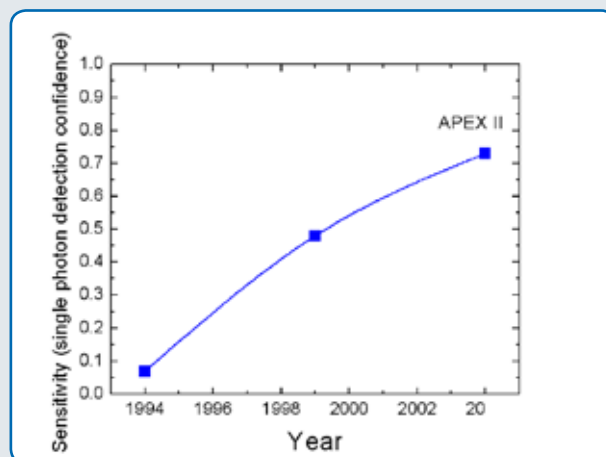


Figure 5: Increase of sensitivity of CCD detectors.

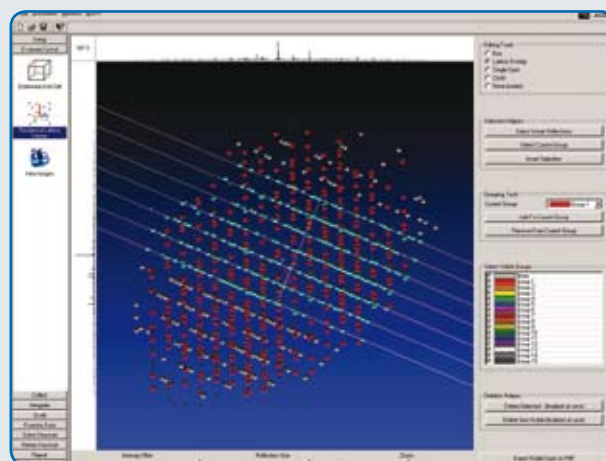


Figure 6: Reciprocal lattice viewer.

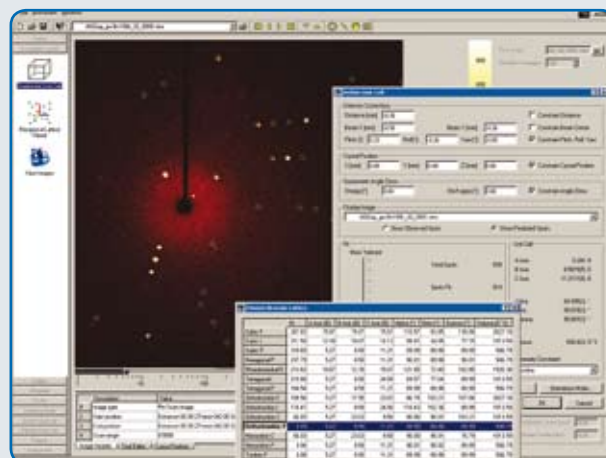


Figure 7: Unit cell determination.

Since 2002 we have benefitted from the tremendous improvement in technology of the CCD chips and have the excellent APEX II detectors available for upgrading the KAPPA CCD systems now.

However, there is still a large number of original KAPPA CCD detectors installed. On one hand we are very pleased to see the detectors we have supplied you with are successfully used in your daily business. On the other hand these systems, which are now between 8 and 14 years old, might not be 'state of the art' anymore. Table 1 compares the technical specifications of the KAPPA CCD and the APEX II detectors. The latter clearly outperforms the KAPPA CCD detector from the specification point of view. This technical superiority is reflected in significantly better data in particular for the high angle data (Figure 1), which in turn provides better crystallographic models.

As you can see the improvement is most significant for the high angle data.

- Take your KAPPA CCD system to the highest level of data quality.
- Increase your productivity with the most sensitive CCD detector available.
- Collect data on even smaller and more weakly diffracting crystals.

Take the benefit from the newly introduced 30 Watt Micro-focus X-ray sources (I μ S), which are available in single and dual wavelength systems, called APEX II QUAZAR and APEX DUO, respectively. Our users running small or weakly diffracting crystals on systems equipped with these sources see a diffracted signal similar to that obtained from traditional rotating anode based systems.

Table 1: Comparative Specifications

Comparative Specifications		
	KAPPA CCD	APEX II upgrade
Active area	90 mm diagonal	90 mm diagonal
Pixel size (μ m)*	55.6	15
Demagnification	2.5:1	1:1 (None)
Spatial distortion	<6%**	0%
Standard frame sizes (pixels) (binning)	1152x1242 (1x1) 576x621 (2x2)	1024x1024 (4x4) 512x512 (8x8)
Readout rate (max, kHz) (binning)	430 kHz 200 kHz normally used	2100 (4x4) 1600 (8x8)
Frame readout (s) (binning)	3.6 sec (1x1) 1.8 sec (2x2)	0.3 (4x4) 0.15 (8x8)
Quantum gain (electrons/x-ray, Mo K α)	11 (until 2002) 18 (from 2002)	170
Antiblooming	No	Yes
Computer interface	Analog	Digital
Point spread function (FWHM) (μ m)	150	75

* at front of detector, unbinned

** software corrected

All configurations and specifications are subject to change without notice. Order No. DOC-H86-EXS010.
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