

PEAK

Electron Spectroscopy Control and Acquisition Software

PEAK is designed to control acquisition of photoelectron spectra with Scienta Omicron analysers. With its modern software architecture, PEAK offers improved performance for data acquisition, work flow, and live visualisation of data. The modular design and the modern network based application programming interface (API) facilitate integration of additional equipment as well as full integration of the analyser in external control systems.

The drive to gain a complete descriptive model of materials and reactions, pushes photoemission spectroscopy experiments to extend into dimensions such as time, space, pressure, and temperature. This causes ever increasing data rates and complexity. At the same time, software standards and architectures have progressed and offer improved support for complex experimental setups and high data rates. With PEAK these advances materialise as efficiency gains and improved work flows, available for Scienta Omicron analysers.



Benefits and Properties:

- Flexible live data visualisation
- Supports high data rates
- Improved work flows
- Network based API for integration with external control systems
- Based on modular architecture

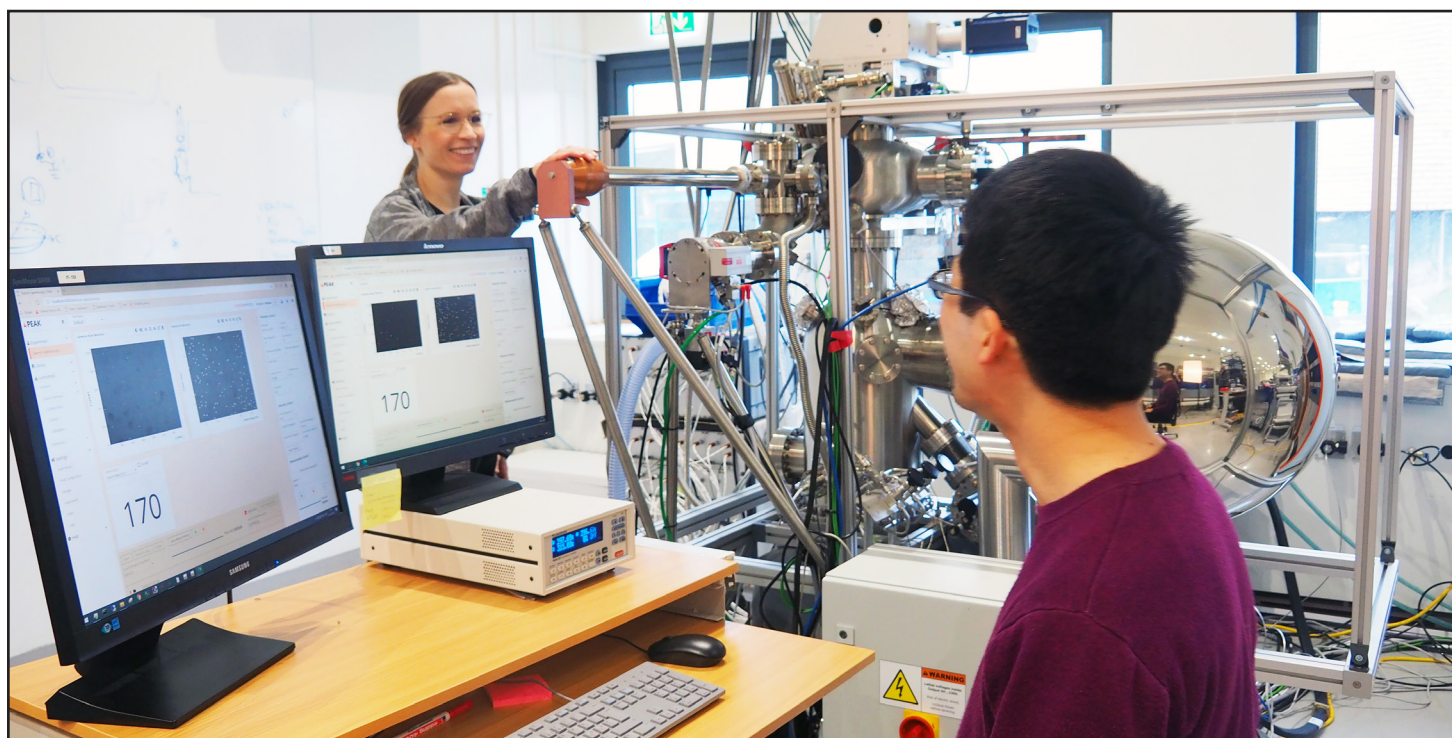


Figure 1: The ARPES Lab is a fully integrated system solution including vacuum system and bakeout capability. This system is configured to have a DA30-L with electronic deflection, narrow band width VUV5k helium ECR based lamp, preparation chamber, and 5.5-axis closed cycle 10 K manipulator. Lowest residual fields at the sample are provided by a double mu-metal shielded chamber. PEAK is used to control both analyser and manipulator and allows early and flexible visualisation of acquired data.

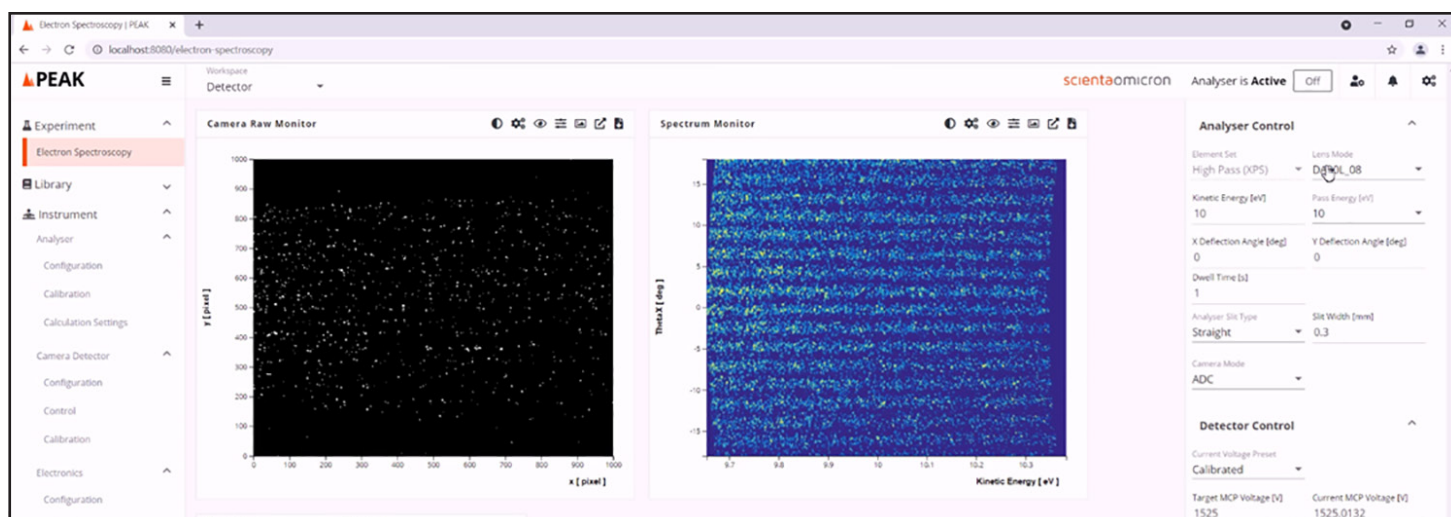


Figure 2: The PEAK graphical user interface controls the analyser. Data windows shown can be adapted to the individual preferences. A camera raw monitor is available without any image corrections, as well as a spectrum monitor with image corrections applied. Displaying, for example, a running average of the data or changing the colour scheme for better visualisation is supported. The analyser control settings are conveniently displayed to the right and easily changed while setting up a measurement. Multiple interfaces can be opened at the same time and displayed across multiple screens.

Graphical user interface (GUI)

The PEAK GUI is accessed through standard browsers and uses network communication to control the analyser hardware. Multiple browser tabs of the GUI can be distributed across multiple screens, ensuring all important information for an experiment can be displayed according to individual requirements.

The main view, as shown in Figure 2, can be configured to show for instance the camera raw monitor directly from the detector without any image processing or corrections applied. A second optional display shows the spectrum monitor. In this view, electron hits from the raw image are processed with either ADC or pulse mode and mapped into the correct spectral channels. The spectrum monitor is continuously updated as more data is accumulated. A convenient feature is to display a running average of accumulated data while fine tuning the analyser parameters. This offers reduced noise and immediate feedback of the attainable data with the currently selected parameters. Each data display can be brought to a dedicated tab by a single click offering an enlarged view of the data, as shown in Figure 3.

Data visualisation

In PEAK, data visualisation is independent of ongoing acquisitions and is therefore fully flexible. Selecting a specific slice of the multidimensional data is done by defining the axes and ranges to be visualised. One can switch between 1D and 2D representation. It is also possible to zoom in on an

interesting region of the displayed data using the mouse. All of this is possible live in the spectrum monitor without interfering with the ongoing acquisition.

For instance, it is possible to display an ongoing deflection scan as a θ_x, θ_y image for a selected slice of energy. With the display continuously updating with new data, it is possible to monitor the signal to noise ratio with each consecutive loop over θ_y deflection and get an early impression of the data. Acquisitions can be stopped directly after each completed step, for instance after loop is completed or after a spectral region acquisition is finished.

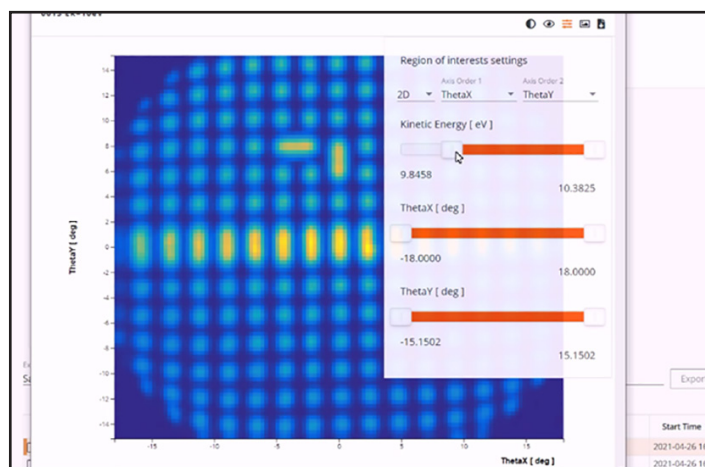


Figure 3: Data visualisation is done on the fly and can be applied to a selected slice or the complete data range. The visualised data is continuously updated as the measurement progresses allowing to explore data without interfering with the acquisition.

Analyser control

The live analyser settings are shown on the right side in the GUI, see Figure 4. Here one can set the lens modes, kinetic energy and pass energies and immediately observe the applied changes in the live spectrum monitor. During measurements, such as an electronic deflection scan perpendicular to the slit, the θ_y deflection must be continuously changed while acquiring data. It is possible to track and monitor the live analyser settings during such a measurement as the analyser control is updated accordingly.

While the analyser control can be hidden, the analyser state is always visible at the top right. Even when the central part shows a settings /calibration dialogue without live data displays, it is always clear if the analyser is ready (off), active (on), or acquiring. The analyser is of course easily turned off manually if required during an ongoing measurement. It is also possible to turn the analyser off from a sequence of measurements as well. This is particularly useful when for example running long unsupervised, overnight HAXPES measurements series.

Detector control

The detector control, as shown at the bottom of Figure 4, allows to quickly adjust or turn off the detector by controlling detector voltages manually. This is useful when conditioning the MCP after venting and allows to easily increase the voltage while observing the live image and count rate. It is possible to store and recall different detector voltage presets. For instance, HREELS or laser ARPES measurements may require low MCP voltages during the setup phase to avoid MCP ageing due to high signal intensities. Once setup is complete, signal intensity is normal and it is easy to switch back to the calibrated detector voltages.

Sequences

A measurement is typically composed of a sequence of steps with acquisitions. PEAK provides a versatile sequence editor in which steps such as loops and spectral regions can be combined in a nested tree structure. When a completely new spectral region is added it inherits the parameters set in the live analyser control and currently used for the data displayed in the live spectrum monitor.

Spectral regions and entire sequences can be stored to and recalled from a sequence library allowing for quick

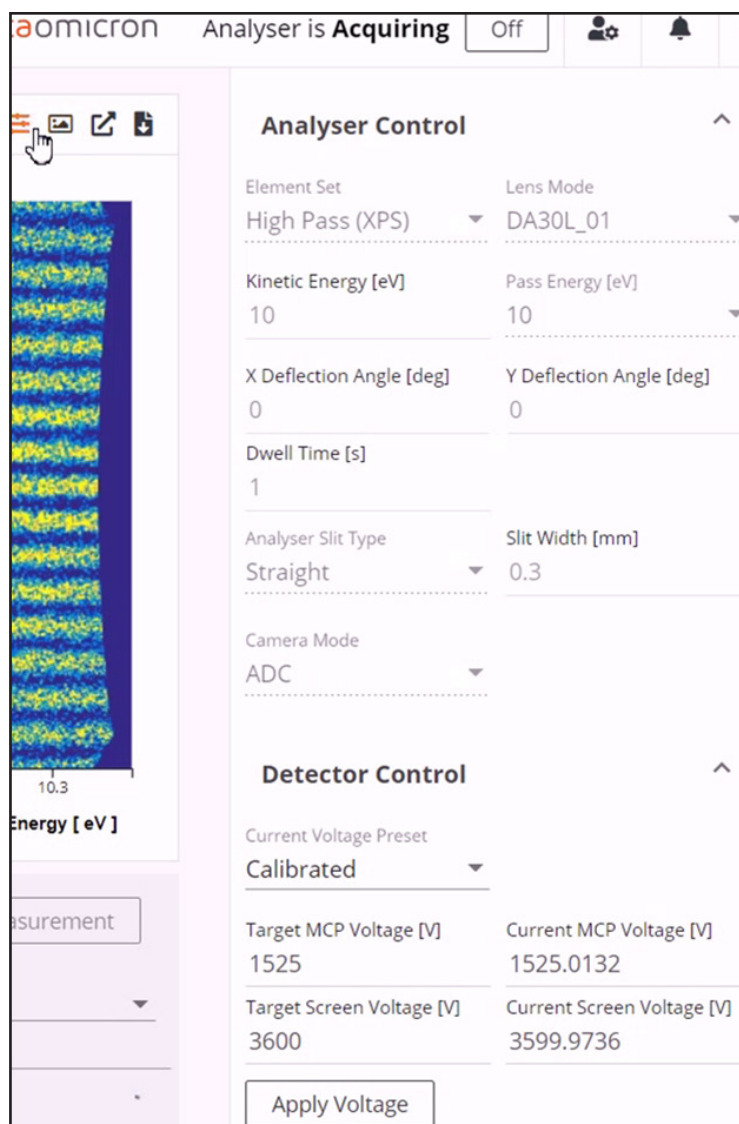


Figure 4: The analyser control panel is easily accessible and gives a live overview of current analyser settings updated while acquiring. During setup different settings are tested and these are readily imported when adding a new spectral region to the measurement sequence.

access to standard measurements such as a XPS overview scan or a check for surface contaminations.

When a measurement is started, the remaining time and number of iterations in the ongoing acquisition are updated and displayed. In the interactive mode additional spectral regions can be added as the experiment progresses. The data in a sequence is stored per spectral region including time stamps which allow to sort and keep track of each spectra during the analysis phase. Once the measurement is finished spectra can be exported automatically (IgorWave, IgorProject, EnergySpectrumCSV, amongst others).

PEAK architecture

Most experiments require controlling a large number of components (sample manipulator, delay stage, pulsed gases, beam lines) while logging sensor data together with each corresponding spectrum. The combination of spectra with auxiliary data is a prerequisite to characterise processes and materials in terms of electron dynamics, chemical reactions, or spatial mapping.

Experimental setups exhibit a great variety of individual requirements depending on the supported measurement techniques. To support the inclusion of new functions, PEAK is based on a modular architecture, see Figure 5. Each individual hardware component is controlled through a dedicated PEAK server. Some of these PEAK servers are written generic and allow the inclusion of a custom user driver. A use case is the PEAK manipulator server which natively supports manipulators controlled through Mistral as delivered with Scienta Omicron system solutions. For a manipulator which is not natively supported, it is possible to write a custom driver which is then plugged in to the PEAK server. The manipulator is then exposed through the PEAK API to the graphical user interface or to an external control system.

PEAK user scripts

Besides user drivers, special regions where user written python scripts are added and executed as part of the measurement sequence is supported. This will for instance allow easy readout or control of additional sensors and logging the meta data with the corresponding spectrum. With this option, PEAK offers a very broad and open interface while lifting the effort of controlling the entire sequence from the user.

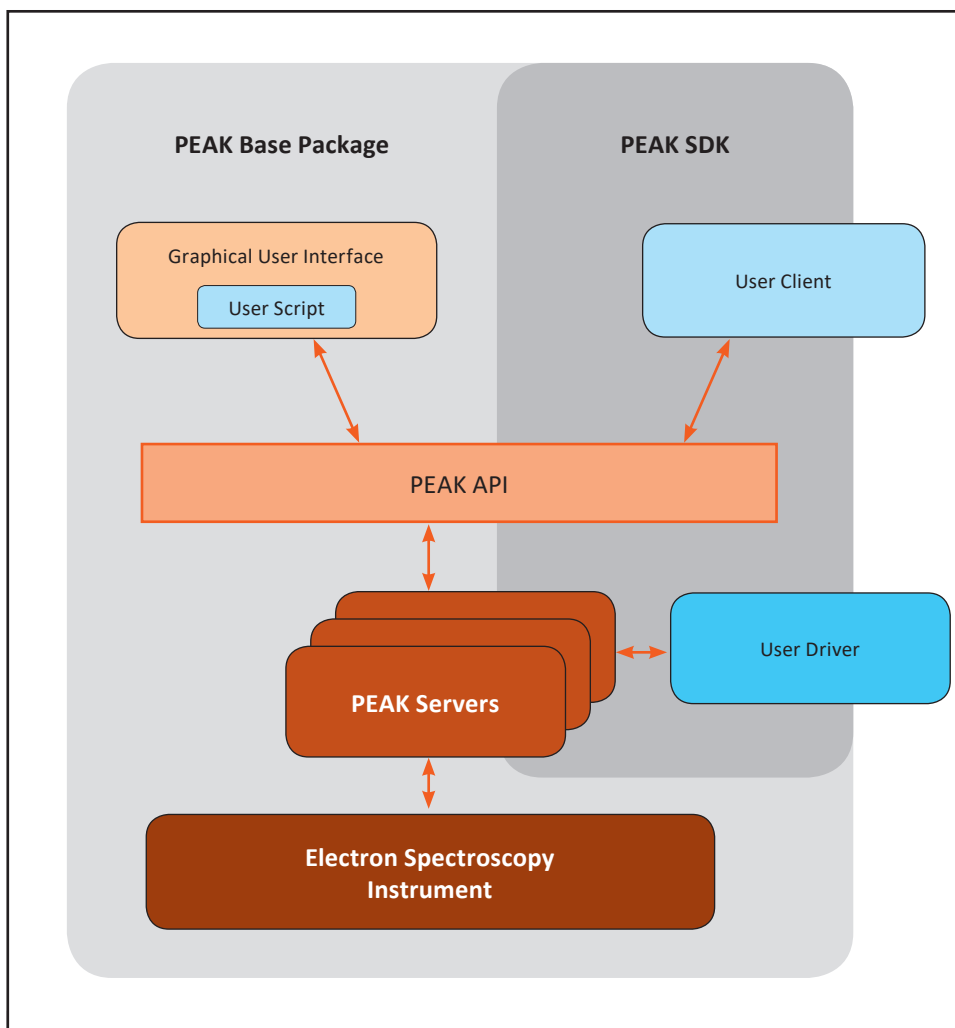


Figure 5: All user interaction, be it through the GUI or using a remote user client, is channelled through the PEAK API using standard network communication. The API accesses the underlying modularised servers. These control either individual hardware components or the experiment logic synchronising the individual hardware components needed to acquire a sequence of measurements.

PEAK API for external control systems

While PEAK can handle setups with various components, distributed control systems (DCS), such as EPICS and TANGO, are commonly used to establish a client-server model as the scale and complexity of a setup increases. The PEAK API is designed with DCS in mind and supports the client-server model with a modern network based communication interface.

The client side can be implemented in a variety of languages such as TANGO, EPICS, Python or LabView. This allows

to control the analyser acquisition from outside of the instrument PC and without requiring hardware driver routines. With this client server model it is even possible to run a DCS concurrent with the use of the PEAK GUI. Hence, while the analyser is controlled through the external DCS the PEAK GUI can for instance display the live analyser settings and the live spectrum monitor. This can be especially helpful during development to verify the expected behaviour.

PEAK SDK & API Training

The PEAK software development kit (SDK) is solely for software development and can by itself not control any hardware. The development environment includes dummy drivers, emulating the various hardware servers, which are controlled through the regular PEAK API. This enables offline development and testing of clients without blocking the analyser hardware from acquiring real measurements. The training course includes an introduction to the architecture, example demonstrations, and exercises for developing clients for the PEAK API. This course is highly recommended when the analyser is to be integrated in an external control system or before writing user drivers.

As the PEAK GUI itself builds on the PEAK API, it is possible for a control system to have the same detail level by addressing the underlying PEAK servers through the API. For low level functionality it is for instance possible to address the camera detector server. For most use cases, it will be far more interesting to focus on higher level functionality provided by the experiment server. It allows an operator to setup and acquire a spectrum region without having to know details of other hardware servers. The acquired data is then returned to the client through the network protocol.

PEAK modules

PEAK is subject to a license agreement and is delivered with a license dongle for the base module which supports control of the analyser and conducting measurements. In a system solution or component bundle from Scientia Omicron, licenses for controlling other supported hardware are included.

With the open interface for user drivers and the inclusion of user written python scripts from the PEAK GUI it is always possible to incorporate hardware components without currently existing PEAK modules. Flood guns, ion sources, or delay stages of other brands can for example be controlled during the measurement with python scripts written by the user or with the support by Scientia Omicron.

Add analyser region to definition (created from spectrum definition)

```
In [21]: measureSequence = experiment.getMeasureSequence()
In [22]: newSequenceRootId = measureSequence['RootId']
In [24]: analyserSpectrumRegionId = experiment.addAnalyserSpectrumRegion(newSequenceRootId)
spectrumDefinition = {
    'Name': 'DA30_01_TestSweep',
    'LensModeName': 'DA30L_01',
    'PassEnergy': 10.0,
    'FixedAxes': {'X': {'Center': 10.0}},
    'SweepAxes': {'Z': {'Offset': -14.75, 'Delta': 0.5, 'Count': 60}},
    'UseCamera': True,
    'Detectors': ['Camera'],
    'CameraMode': 'ADC',
    'DwellTime': 1.0
}
experiment.setAnalyserSpectrumRegion(analyserSpectrumRegionId, spectrumDefinition)
```

Acquire (perform measurement)

```
In [25]: experiment.acquire()
```

Finish measurement (stores measurement made from sequence definition to storage)

```
In [26]: experiment.finishMeasurement()
```

Export and get the spectrum

```
In [27]: storage.clear_exports()
sequenceLog = storage.get_sequence(sequenceLogId)
firstAcquisitionLog = sequenceLog.acquisition_log(0)
firstSpectrumLog = firstAcquisitionLog.spectrum_log(0)
spectrum = firstSpectrumLog.spectrum();
```

Show the spectrum

```
In [28]: fig, ax11 = plt.subplots(1, 1, figsize=(10, 10))
spectrum.show_plane(ax11, 2)
```

Figure 6: Conducting an acquisition using the PEAK API does not require intricate knowledge of all involved servers. It is sufficient to define the spectrum properties and request the acquisition, as shown here with Python.

Upgrading from SES to PEAK

PEAK is available as an upgrade to DA30-L, EW4000, R4000, and other Scienta Omicron analysers, which were originally delivered with SES and the SESWrapper for server-client communication. To ensure a good transition, PEAK supports import of the current SES instrument calibration data, and remote support is included for the software installation. Parts of the analyser electronics, detector and computer may need to be upgraded to be compatible with PEAK and PEAK ready hardware upgrade packages are available.

With a PEAK upgrade, the service life of previously installed analysers can be substantially extended and access to new software functionality is possible. While SES is supported with its current scope, development of new functionality is focused on PEAK. These include support for new detectors and integrating new equipment with the data acquisition, as well as software improvements.

Auxiliary components

When upgrading an entire setup it is also important to consider the complete configuration including required measurement functionality and auxiliary components such as manipulators or a delay stages. Components are supported in PEAK through user scripts, user drivers, and external control systems. Please contact your service representative to find a suitable solution how and when to optimally transition from SES to PEAK.



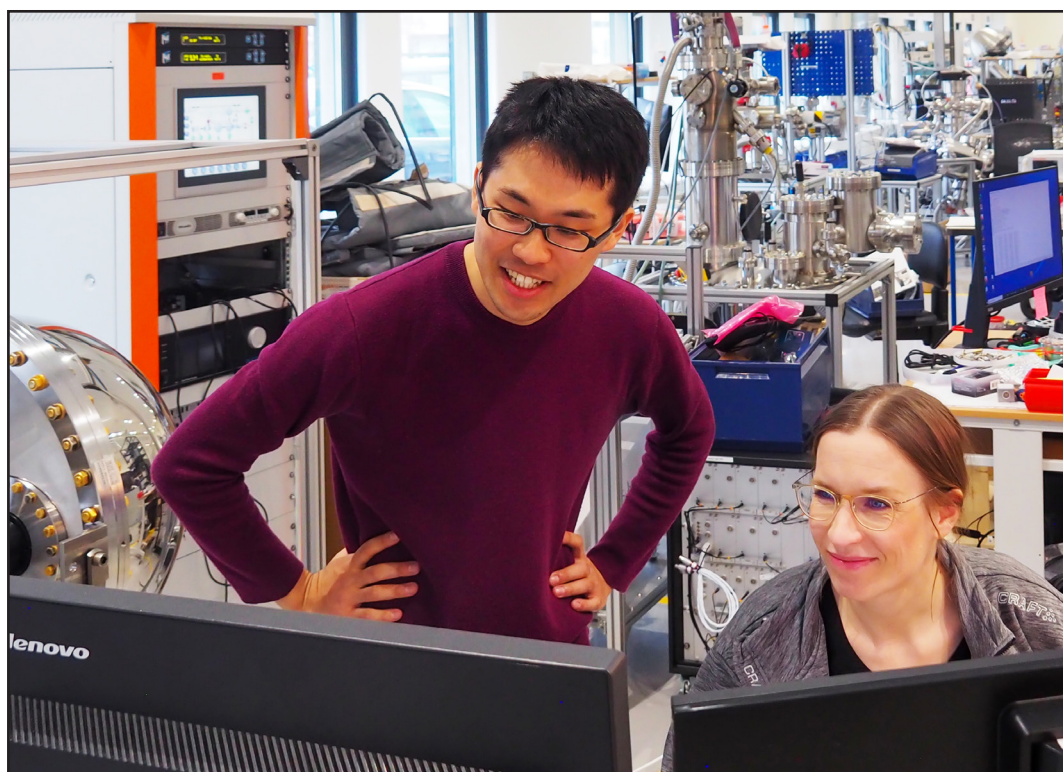
Figure 7: The analyser control upgrade package brings the HV rack communication, detector camera, and the instrument PC to the latest standard. With this the PEAK minimum requirements are satisfied and extend the life of older generation analysers.

Scienta Omicron provides PEAK ready service packages ensuring:

- Analyser hardware compatibility
- Upgrade of HV rack to ethernet communication standard
- Upgrade to compatible and fast detector camera
- Upgrade to preconfigured and high performance Win10 based instrument computer
- Evaluation of other hardware component requirements

PEAK outlook

PEAK supports most our hemispherical analysers with more hardware support being added constantly. Additional features and modules are being developed in PEAK with functionality not even possible to implement in the SES architecture. Check with your local Scienta Omicron representative for the latest updates.



Technical Data

PEAK

Flexible data visualisation during acquisition
Versatile sequence editor
Comprehensive logging of metadata with each spectra
Supports high frame rates
Auto export of measurements

PEAK API

Network based client-server communication
Programming language independent (Python, TANGO, EPICS, LabView)
Control of low & high level functionality
External control concurrent with use of PEAK GUI
Software development kit for offline development with dummy drivers

Available for analysers:

DA30-L, DA20, R4000, R3000
SES2002, EW4000

Supported detectors:

MCP/digital camera
DLD (selected models)

Minimum requirements:

Ethernet standard for HV-rack and digital camera
PEAK ready MS Windows 10 Instrument PC

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