KolXPD

software for photoelectron spectroscopy data measurement and processing

Feature Highlights

- Focused to photoelectron spectroscopy
- Very fast data viewing and processing
- Energy- and angle-resolved experiments
- Import and export of variety formats
- Huge amount of data handling
- Fitting, waterfall charts, quantitative preview
- Functionality customizable on request

Charles University in Prague, Czech Republic

Academy of Sciences of the Czech Republic, Prague

Synchrotorn Elettra Trieste, Italy

National Institute for Materials Science Tsukuba, Japan

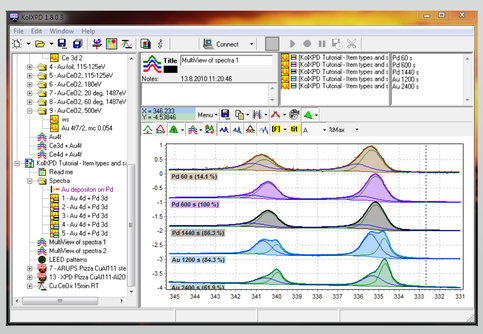
Synchrotorn SPring-8 Sayo, Japan

Heinrich-Heine-Universität Düsseldorf, Germany

most significant institutes where KolXPD is used

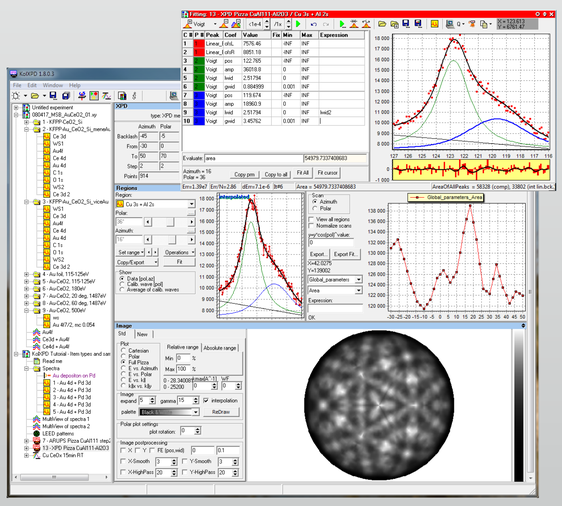
Photoelectron spectroscopy features

- import of data from many analyzer softwares (SpecsLab, Spectra, Omicron, VG, etc.)
- complete XML experiment file of SpecsLab can be loaded and processed, including each region channel and sweep data
- spectra can be acquired by KolXPD (currently with Specs analyzer, others on request)
- support for synchrotron radiation spectroscopy
- spectra can be quickly fitted with most common peak shapes and backgrounds
- all data are organized in one tree structure
- just select more items to view them in one multiview chart
- multiview has many icons for instant processing which doesn't affect original data. Just click to view normalized spectra, make waterfall, subtract background, show fit results, smooth, etc.
- using multiview it is possible to fit dozens of spectra quickly and automatically
- all result data can be exported, all graphs copied into clipboard and pasted anywhere
- data can be transferred in both directions between KolXPD and WaveMetrics Igor Pro for further processing and presentation



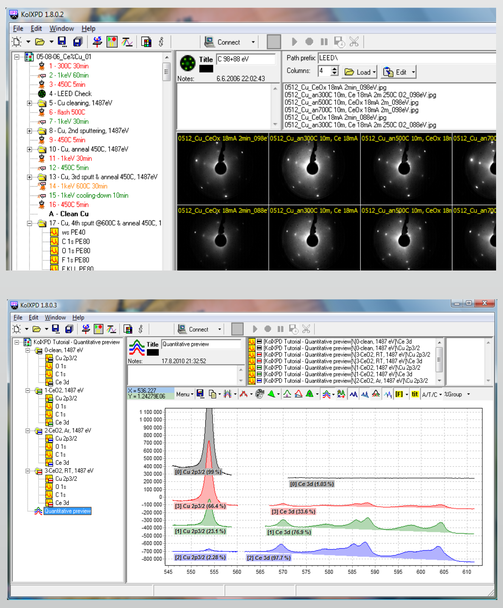
Multidimensional experiments

- support for energy-resolved experiments using synchrotron radiation – methods like NEXAFS, Resonant photoemission, etc.
- support for angle-resolved spectroscopy, e.g. XPD (X-ray Photoelectron Diffraction) and ARUPS (Angle-Resolved UV Photoelectron Spectroscopy - band mapping)
- KolXPD can measure this experiments using analyzer, sample manipulator or beamline monochromator
- 2-dimensional angle-resolved data can be plotted as a pattern picture in Cartesian or polar coordinates
- thousands of 2D experiment spectra can be easily and automatically fitted by one shape
- intensity of each pattern point can be spectrum area or any parameter of fit function
- results of XPD pattern modeling software EDAC can be imported and displayed in same way
- multidimensional data can be imported and exported, including pattern pictures – as both text and image format



Other features

- tree structure is useful for whole experiment handle; other items can be added to describe experiment steps e.g. cleaning, heating, deposition, gas exposure etc.
- you can add own notes to any item; folders and note items can contain HTML-formatted text
- simple image browser e.g. for LEED pictures
- KolXPD allows simple quantitative preview by showing peak areas corrected by analyzer transmission function and photoemission cross-section
- relative concentrations can be showed for each folder; it's useful for preview of concentration evolution during experimental steps
- all files of KolXPD has open text format – you can write an import to your favorite software



Watch video-tutorial at
http://www.kolibrik.net/kolxpd/

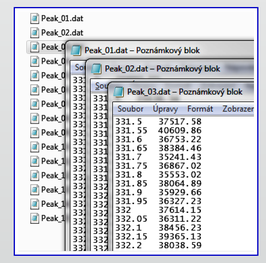
How to import 15 spectra, make graphs, fit peaks and analyze results in 90 seconds !!!

Tutorial steps:

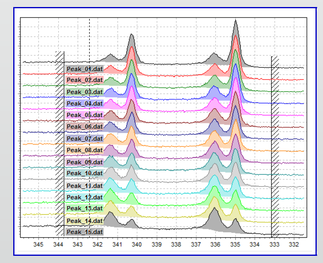
- start: 15 raw XY text files with sample spectra (2 doublets)
- import to KolXPD by single drag-and-drop
- place spectra to one graph, change x-axis to binding energy
- change display to waterfall and color-filled peak area
- define x-axis range and fitting function for middle spectrum
- automatically fit all spectra with this function
- display fit results
- export area evolution of doublets and display in new graph
- fit area evolution with linear function

All this done in 90 seconds!

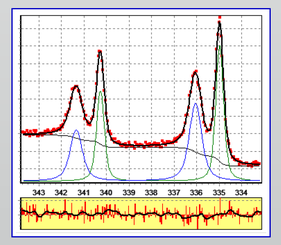
Video snapshots:



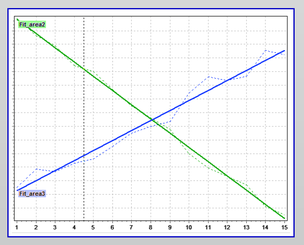
Raw XY text files



Waterfall view in KolXPD



Fitting of one spectrum



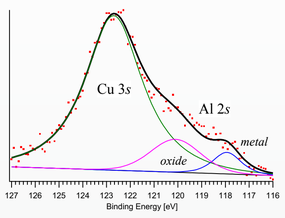
Doublets - area evolution

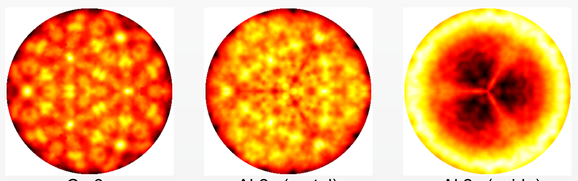
Angle-resolved photoemission experiments

acquired using KolXPD at Charles University in Prague

2D angle-resolved spectra of core-levels and valence band can be measured.
All measured spectra can be automatically fitted and components of fit can be used for displaying a pattern.
Valence band can be displayed as polar or azimuthal plot or as 2D map like Fermi surface map.

$Al_2O_3/Cu_{91}Al_9(111)$





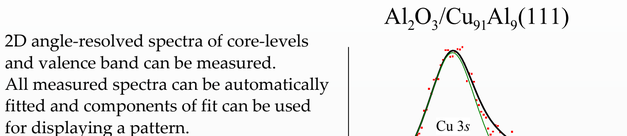
Valence band polar scan

Fermi surface map

XPD pattern calculations made by EDAC*

patterns and clusters can be vizualized by KolXPD

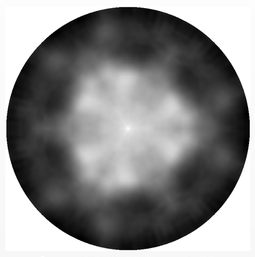
*Software for X-ray photoelectron diffraction (XPD) pattern calculations
F. J. García de Abajo, M. A. Van Hove, and C. S. Fadley, Phys. Rev. B 63, 075404 2001.



Angle- and energy-resolved photoemission experiments

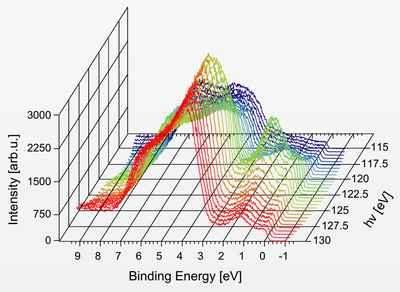
acquired using KolXPD at Materials Science Beamline, synchrotron Elettra

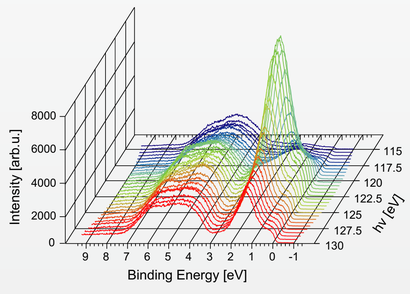
KolXPD can control both manipulator and monochromator – energy-resolved experiments like NEXAFS, resonant photoemission, etc. are possible. Graphs below show resonant experiment on cerium-oxide and XPD patterns acquired at two different resonant photon energies.

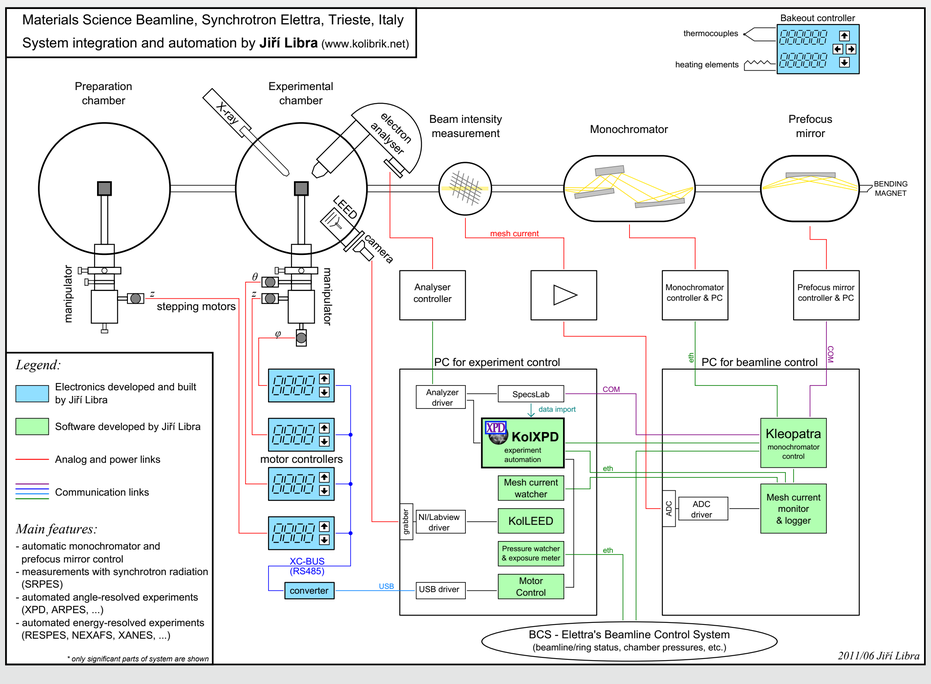


hν = 124.8eV, EB = 4eV

hν = 121.4eV, EB = 1.8eV



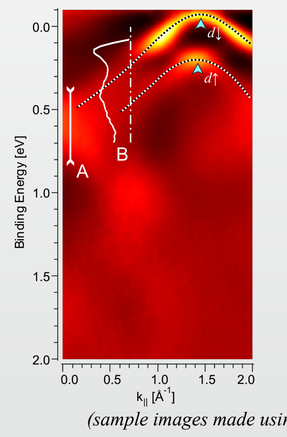




Reference papers and results

where KolXPD was used for measurement and data processing

- **J. Libra**, V. Matolín, Surf. Sci. **600** (2006) 2317
  Angle resolved photoemission study of the Ce/Pd(111) interface
- **J. Libra**, et al., Phys. Rev. B **76** (2007) 165438
  Angle-resolved photoemission study of ordered Pb/Ni(111) surface phases
- V. Matolín, **J. Libra**, Surf. Sci. **601** (2007) 4058–4062
  Fermi surface and band mapping of the cerium/palladium surface alloy
- M. Škoda, **J. Libra**, et al., Surface Science **601** (2007) 4958
  A resonant photoemission study of the Ce and Ce-oxide/Pd(111) interfaces
- V. Matolín, **J. Libra**, et al., J. Phys. Chem. C **112** (2008) 3751
  Photoemission spectroscopy study of Cu/CeO2 systems: Cu/CeO2 nanosized catalyst and CeO2(111)/Cu(111) inverse model catalyst



(sample images made using results of KolXPD data processing)

About author

Mgr. Jiří Libra, Ph.D. *(email: Jiri.Libra@gmail.com)*

- Surface science experienced during 10 years spent in Department of Surface and Plasma Science at Faculty of Mathematics and Physics, Charles University in Prague under supervision of *prof. Vladimír Matolín*
- Business activities: development of software and electronics (not only) for science. Experiment automation, data acquisition and processing, electronics for angle-resolved experiments, software for beamline monochromator control, scientific device interfacing, etc.

KolXPD Web

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