CasaXPS Feature List

CasaXPS represents the state-of-the-art in XPS spectral analysis. Options and procedures in CasaXPS have been developed in conjunction with numerous laboratories working with XPS spectra acquired using almost every instrument available. Close collaboration with experienced XPS analysts means that CasaXPS not only offers a wide range of features, but these features are of practical use on an everyday basis.

CasaXPS is an ISO 14976 (VAMAS) file browser however file conversion filters are available for most file formats allowing users of CasaXPS to process data from almost every instrument in use today.

Quantification

Automatic peak identification
Automatic quantification region creation
Element library driven quantification region creation
Transmission corrected quantification reports
Instrument manufacturers, NPL and user defined transmission functions
Angular distribution corrected Scofield cross-sections
MFP correction
Backgrounds and peak-models defined on region-by-region basis
Monte Carlo determined error bars
User defined quantification report formats
Quantification reports from combination of regions and synthetic lines
Quantification reports based on Intensity calculator
Automatic transfer of quantification to related spectra
Quantification based on peak-to-peak intensities (AES)
Quantification based on survey spectra with intensities proportioned by high resolution scans
Creation of Depth Profile VAMAS files from Quantification Tables.

Chemical State Analysis

Peak-models saved to file
Background types: Linear, Shirley, Analytic Shirley, Kappa parameters Shirley, Two parameter and three parameter Tougaard, Cubic Spline mouse adjustable backgrounds, Max, Min, Mean, Zero, Smoothed
Peak fitting with linked constraints
Line-shapes: Gaussian Lorentzian sum and product, Voigt function, asymmetric tail to GL functions, Doniach Sunjic, Gelius, hybrid GL/Doniach Sunjic
Line-shapes defined from spectra
Optimisation: Marquardt, Simplex
Peak constraints spanning elemental acquisition regions
Monte Carlo error estimates for peak fitting parameters
Peak-fit spatially resolved spectra; Creation of Chemical State Images
Element library markers: periodic table and energy ordered scrolled list

Processing

Processing history saved to file
Smoothing: Savitzky Golay quadratic, quartic and linear, Gaussian, Optimised envelope
Differentiation Savitzky Golay
Integration Savitzky Golay

Linear based depth profile analysis: PCA TFA Linear Regression
Energy Calibration: individual and depth profile layer adjustments based on regions or synthetic components
Intensity Calibration: MFP and transmission correction to spectra, import of transmission functions (NPL)
Spectrum Calculator: general arithmetic expressions in terms of spectra, global operator/operand calculations.
Normalisation of Spectra
Interpolated spectra
Spike removal
Satellite subtraction
Propagate spectrum processing

Annotation

Annotation History saved with each spectrum
Text with line pointer
Chemical Formulae
Quantification table based on regions
Quantification table based on synthetic components (with and without constraints)
Peak labels created from Element library
Propagate spectrum annotation

Display Options

Mark and click to zoom
Zoom list cycled under mouse control
Reset zoom list with quantification regions
3D montage
3D projection from factor space
Overlay stack of spectra
View transmission curves
User selected fonts and colours: axes labels, header information, title
Dashed lines for synthetic components
Dashed lines for spectra
Description key for overlaid spectra
Numerous switches for toggling on/off display items
Residual plot
Background subtracted spectra

Toolbar buttons for adjusting view port into spectrum
Mouse and function key accelerators
Save current display options between sessions

Export Options

Clipboard data transfer
Tab delimited spectra, background, components and total synthetic envelope
Simplified (ISO 14976) VAMAS files
QUASES two column output

SIMS Features

Isotope library
Exact Mass Calculator linked to isotope library
ToF SIMS time-to-mass calibration
SIMS specific display options: zoom to zero baseline, log scale, step by unit mass, preset mass ranges

File Format

ISO 14976 (VAMAS) file format exported by:
SPECSLAB II (copy and paste data transfer)
Kratos Vision 2.x
Service Physics (SSI M-Probe)

Merge VAMAS files on input

CasaXPS offers many edit modes for enhancing quality of information in VAMAS files.

File Conversion Options

CasaXPS offers a common data processing package for a wide range of instruments. Many file formats are easily converted to the ISO 14976 file format read for analysis in CasaXPS.

XPS

SPECSLAB I .exp files
PHI Multipak binary files (including transmission function)
VG Eclipse binary files (including transmission function)
VG Avantage ASCII export files
Kratos DS800 binary files
SSI M-Probe binary files
Scienta DOS binary files
Scienta Windows NT binary files (transmission function on conversion)
RBD Enterprises (copy and paste data transfer)
Bristol Interface Analysis Centre (John Day)
VGX900/Omicron/VSW Ltd/Spectra(Ron Unwin) ASCII files
X,Y pair ASCII files (regular and irregular energy steps)
Quick Scan Ltd files
New file import filters on request

SIMS/ISS

RBD Enterprises
PHI TRIFT II .tdc .sur binary files
Ion ToF ASCII files
Millbrook Instruments Ltd
Hiden ASCII Quad SIMS
Leybold ISS

Support

Direct support from the author of CasaXPS is actively encouraged.