Combined XPS and XAS Analysis Using the Software UNIFIT 2013

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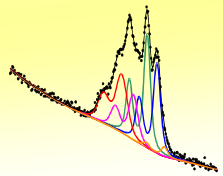


Abstract: A combination of X-ray absorption spectroscopy (XAS) and X-ray photoelectron spectroscopy (XPS) using synchrotron radiation with variable energy and polarized soft x-rays with high resolution and high flux is a powerful technique to observe atomic compositions and electronic state of surfaces of materials. In order to extract the maximum of information of the studied material a spectrum fit for both methods has to be done. The newest version of the software UNIFIT allows the combined spectrum processing and peak fit of XPS and XAS measurement data. The different theoretical description of the spectral background of XA spectra was implemented in the software. Additionally, the input routine was expanded for the reading of four special XAS data formats (NEXAFS, BESSY-EMP/2, LUND-MAXlab Scan Zeiss, 1. Column: Photon Energy - 2. Column: Intensity). The peak fit of a XA and XP spectrum of Ti 2p as well as an XMCD study of a thin Co film on $BaTiO_3$ demonstrate the new possibilities of the improved software UNIFIT 2013.

THEORY

1. Modeling the Peak Form

XPS

The peak form of XP spectra can be modeled using a combination (product, sum, convolution) of a Gaussian and Lorentzian (in case of asymmetry: Doniach-Sunjic peak form) function. The XPS peaks may show asymmetry at the low kinetic energy side (normally displayed on the left hand side).

XAS

The peak form of XA spectra can be modeled using a combination (product, sum, convolution) of a Gaussian and Lorentzian (in case of asymmetry: Doniach-Sunjic peak form) function. The XAS peaks may show asymmetry at the high photon energy side (normally displayed on the right hand side).

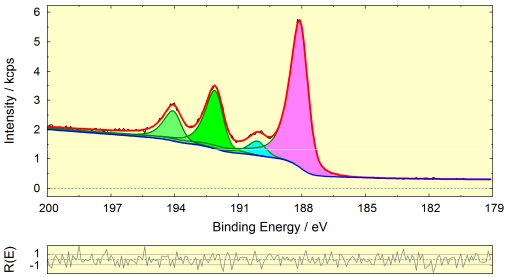
2. Modeling the Spectral Background

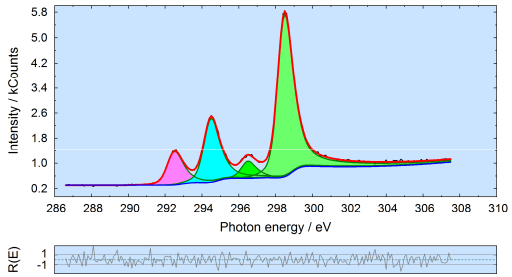
The universal description of the spectral background of XP spectra is the combination of a polynomial, a Shirley- and a Tougaard background with an adjustable Inelastic Electron Scattering Cross Section.
Example background consists of:

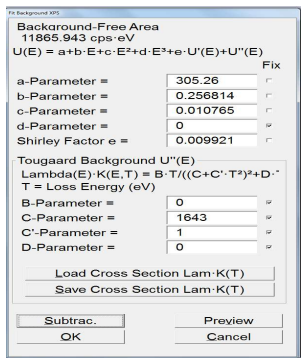
- **one** polynomial
- **one** Shirley step function

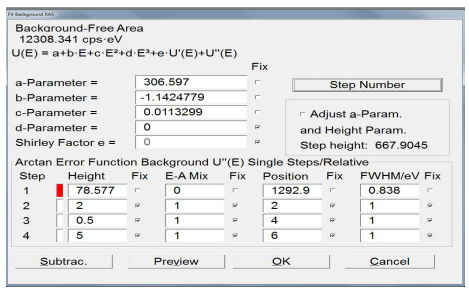
The spectral background function of XA spectra with **n** corresponding XPS peaks can be modeled using a combination of **n** polynomial functions plus **n** mixed Arctan-Error functions.
Example background consists of:

- **four** polynomial functions
- **four** arctan-erf step functions





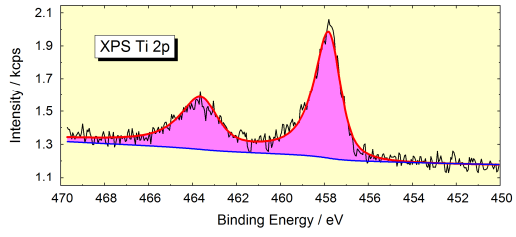


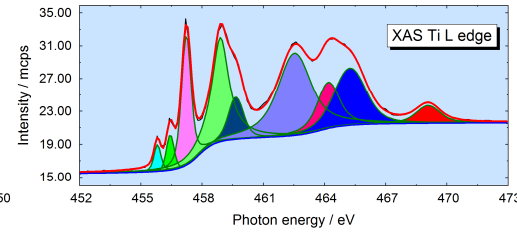


EXAMPLES

Example 1: Combined XPS and XAS Analysis of Ti 2p and Ti L edge

Both the Ti 2p XP spectrum and Ti L edge XA spectrum were recorded. The fit parameters (height, Lorentz-Gauss mixing (sum), peak position, FWHM) of the peak fit of the XP spectrum was introduced into the fit parameters of the spectral background of the XAS spectrum.





Doublet name Ti 2p_XPS 1 Dublett	Peak height/ cps	Lorentzian	Position/ eV	FWHM/ eV	Asymmetry	abs. Area/ cps eV	rel. Area/ %
Doublet 1	768.023	0.723	457.82	1.43	-0.1	1626	67.26
	0.38	1	5.83	1.42	1	791	32.74

Arctan Error Function Background U''(E) Single Steps/Relative

Step	Height	Fix	E-A Mix	Fix	Position	Fix	FWHM/eV	Fix
1	0.005		0.723		457.82		1.43	
2	0.38		1		5.83		1.42	

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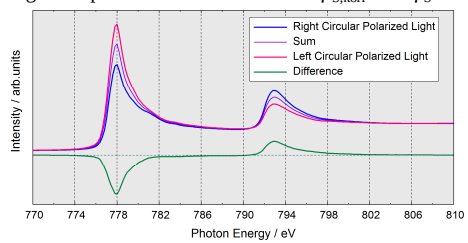
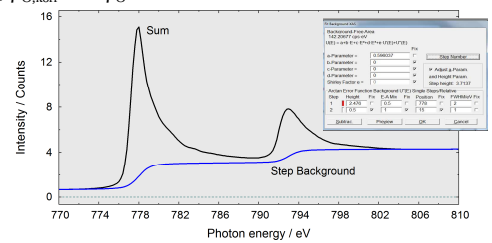
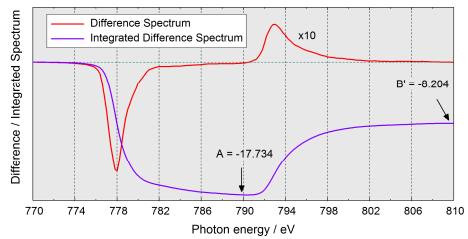
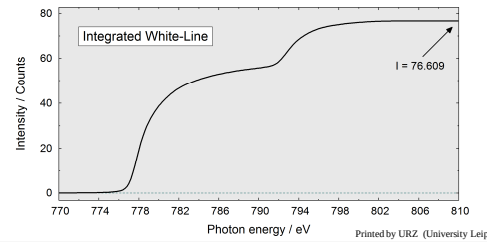
Example 2: XMCD Analysis

The magnetic moment of a thin Co film (21 mono layers) on $BaTiO_3$ using a XMCD experiment of a Co L edge has to be calculated. The sample was excited with left and right circular polarized light. The magnetization direction was in-plane. Derived values: step height: 3.714, N = 2.49 (number of d holes), C = I/N = 30.767, B = B'–A = 9.53, μ_S = -(A-2B)/C, μ_O = -2(A+B)/3C. After correction (X = I/(0.95·sin50°) = 1.37, 95% polarized light angle: 50°) we calculated the magnetic spin and orbital moment to: $\mu_{S,korr} = X \cdot \mu_S = 1.642$, $\mu_{O,korr} = X \cdot \mu_O = 0.245$.









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