Hard X-ray Photoelectron Spectroscopy up to 14.5 keV on Au and C and $YBa_2Cu_3O_{7-\delta}$ Single Crystals

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Scientific Motivation

- Increase XPS Probe Depth
- High Energy Resolution in VB-Spectroscopy (High Resolution with Crystal Monochromators)
- Combination with Diffraction (e.g. X-ray Standing Wave Investigations on YBCO)

Experimental Motivation

General

- High monochrom. flux now available
- Possibility of focussing undulator radiation without too much loss

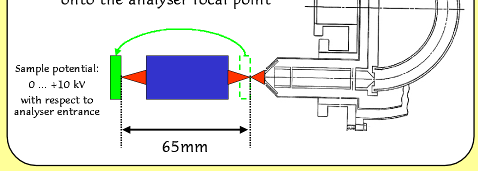
Our Project

- Get first experience with min. modification of equipment
- Obtain experimental cross sections for further planning
- Are Scofield-Tables (1973) useful here?
- Try Standing Wave research on YBCO

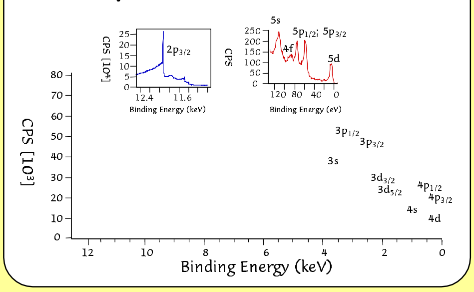
Modification of the PHI-Analyser

Idea:

- Strongly retard photoelectrons by biasing the sample
- Keep the analyser entrance field-free by inserting a matching lens that images the photoelectrons onto the analyser focal point

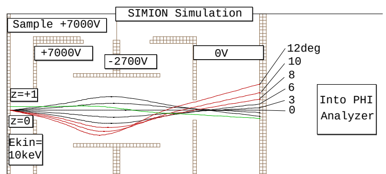


Continuous Spectrum of Au 2p to VB at Eγ = 13.5 keV

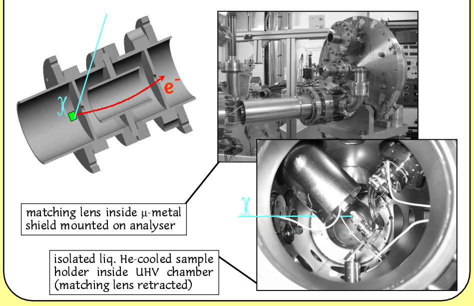


Lens Design with SIMION

Modelling of the photoelectron path: Matching the electron emission solid angle and the source point size to the acceptance of the PHI analyser

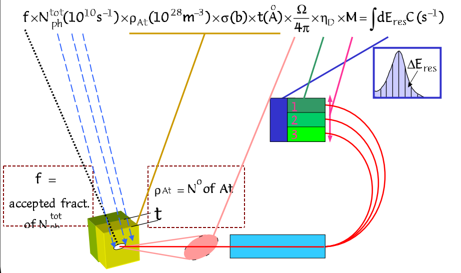


Lens and Sample Mounting



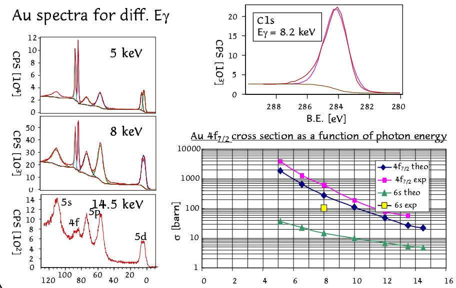
Total Counts in Sub-Level

$$f \times N_{ph}^{tot}(10^{10}s^{-1}) \times \rho_{At}(10^{28}m^{-3}) \times \sigma(b) \times t(\mathring{A}) \times \frac{\Omega}{4\pi} \times \eta_D \times M = \int dE_{res} C(s^{-1})$$



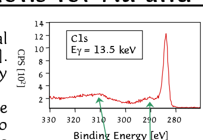
Determination of Cross Sections

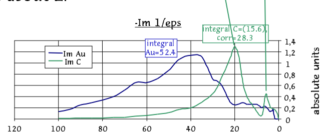
Au spectra for diff. Eγ



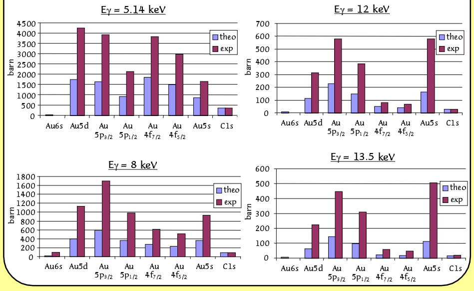
Energy-Loss Functions for Au and C

The Energy-Loss is proportional to Im [1/dielectric constant]. Here it is plotted for glassy carbon.
The integral is corrected for the density of graphite. Its ratio 52.4/28.3 =1.9 confirms t(C)/t(Au) to be about 2.

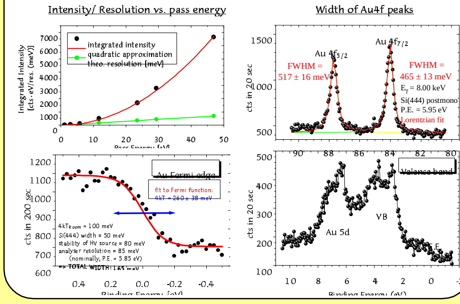




Experimental vs. Scofield H-F-S Cross Sections



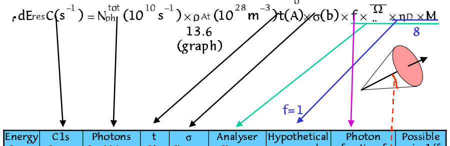
Resolution Tests at Eγ = 8keV



Efficiencies at Pass E. = 46.85 eV

$$\int dE_{res} C(s^{-1}) = N_{ph}^{tot}(10^{10}s^{-1}) \times \rho_{At}(10^{28}m^{-3}) \times t(\mathring{A}) \times \sigma(b) \times f \times \frac{\Omega}{8} \times \eta_D \times M$$

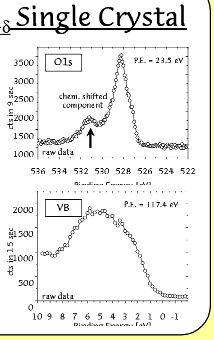
13.6 (graph)

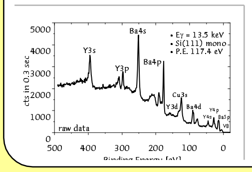


Energy [keV]	C1s [CPS]	Photons [10^{10}/sec]	t [Å]	σ [barn]	Analyser efficiency	Hypothetical cone angle [degree]	Photon fraction f with 6° cone	Possible gain 1/f by focussing
5	155423	515	100	360	0.000077	1.00	0.028	35.6
8	93898	458	140	91	0.000148	1.39	0.054	18.5
10	36779	385	160	47	0.000117	1.23	0.043	23.5
12	14361	178	180	27	0.000153	1.41	0.056	18.0
13.5	5203	160	200	19	0.000079	1.01	0.029	34.8

XPS on $YBa_2Cu_3O_{7-\delta}$ Single Crystal

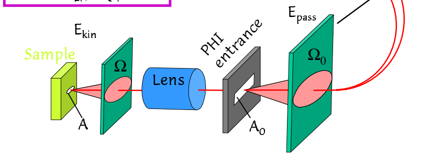
- crystal cleaved *ex-situ*
- room-T
- Eγ = 8.0 keV
- Si(444) postmono (~50 meV energy width)





Intensity Loss (Liouville) Possibilities for Gain

$$Cts/ch \sim A \cdot \Omega \cdot \Delta E_{ch}$$
$$\leq A_0 \cdot \Omega_0 \cdot \frac{E_{pass}}{E_{kin}} \cdot \frac{s_{ch}}{2R} \cdot E_{pass}$$
$$= A_0 \cdot \Omega_0 \cdot \frac{\Delta E_{ch}^2}{E_{kin}} \cdot \frac{2R}{s_{ch}}$$



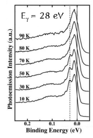
Outlook on XPS/ XSW with Superconductors

XSW

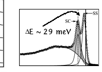
The measurability of high energy photoelectrons allows accessing an uniquely large range of reflection orders. This will represent an unprecedented thorough Fourier analysis applied to the localisation of valence electrons in HTS compounds

XPS

This approach may indicate a way how the superconducting condensate could be localised in the unit cell in an experimentally very direct way. Inevitable signals from surface states can be much reduced.



ARPES of $YBa_2Cu_3O_7$: Opening of the superconducting gap



D. H. Lu, Z.-X. Shen et al., *PRL* **86**, 4370 (2001)