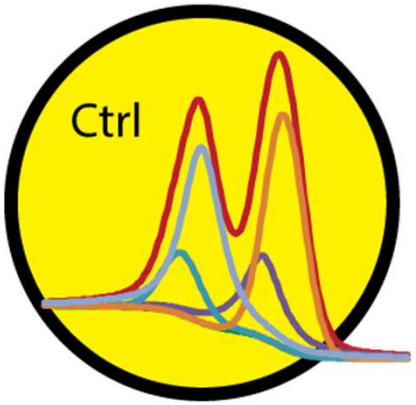


XPS & NEXAFS data analysis suite: Ctrl+Q

- efficient and effective analysis ever experienced -

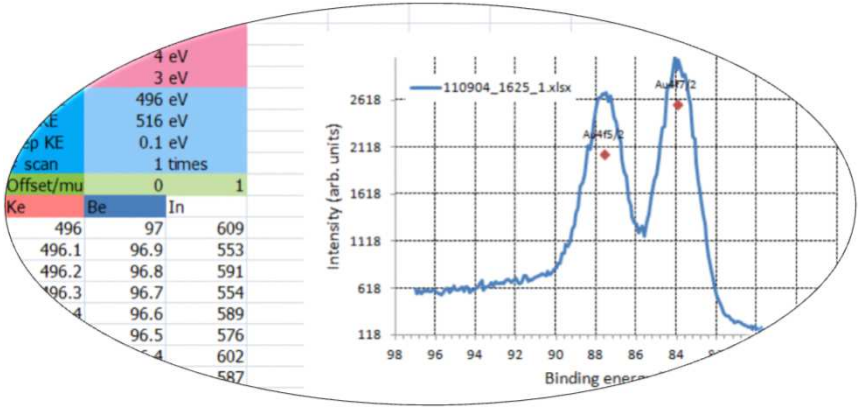
Hideki NAKAJIMA

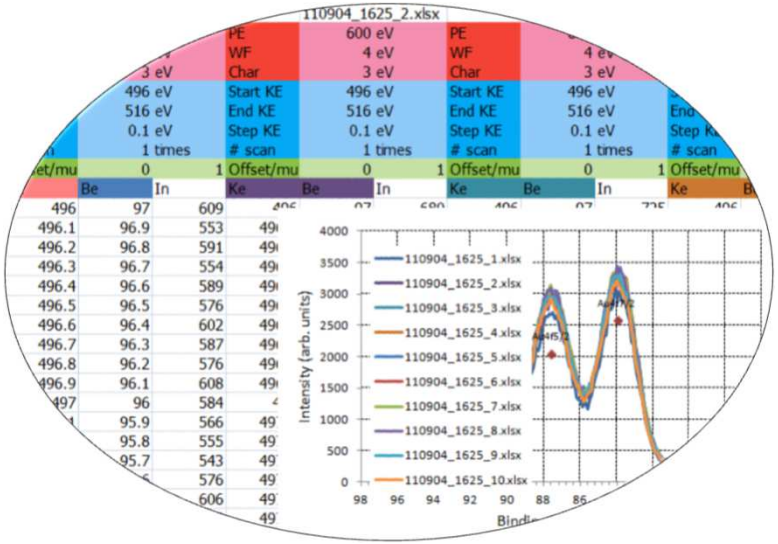
github: heitler/xps-excel-macro

10 May 2019

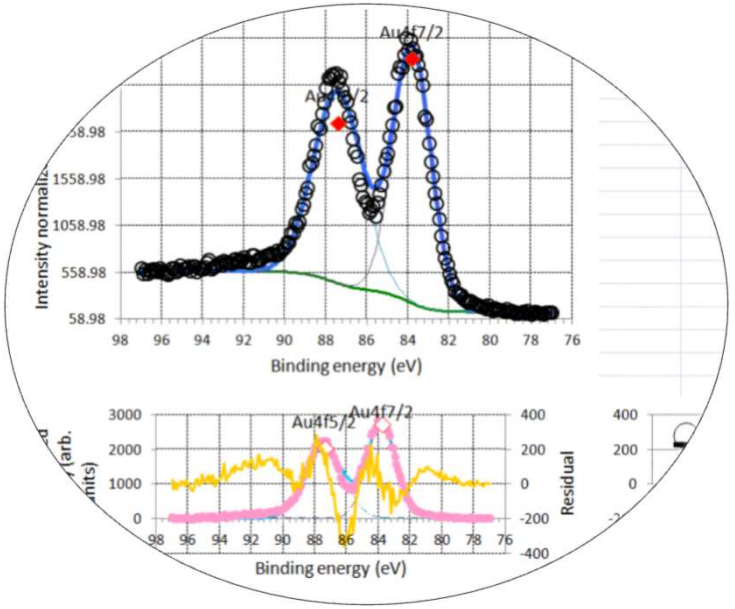
Brief

Plot with binding energy
Identify elements and states





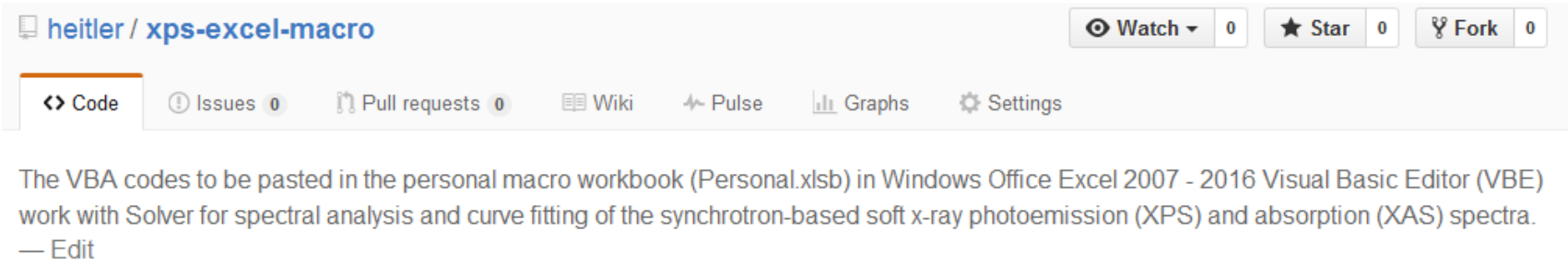
Energy and intensity calibrations



Curve fitting and BG subtraction

Preface

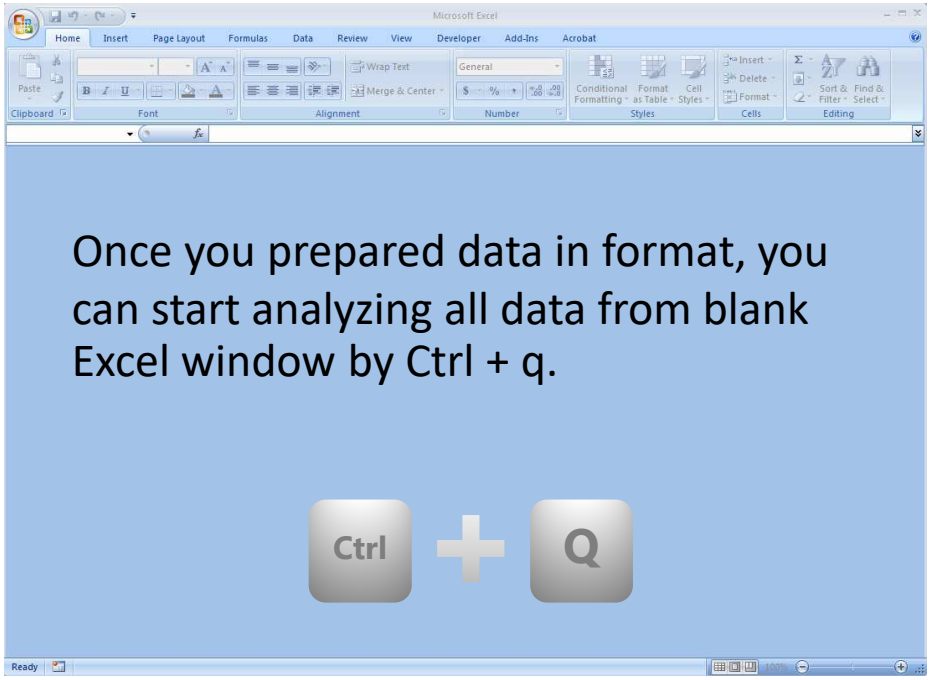
- **Ctrl+Q** is the first comprehensive data-analysis code for **SR**-XPS and XAS working on Windows Office **Excel 2007 or later**. Mac **Excel 2016** works great now.
- Ctrl+Q will analyze the data by just pressing the shortcut key: **Ctrl** + **q**.
- It works great in publication quality.
  - Carbon, JPAP, ASS, ACS AMI, SAB, RCS Adv. etc. from the data obtained at BL3.2Ua and 5.3 in SPL
- **GitHub: xps-excel-macro** for updated info.



Data preparation

	A	B
1	KE/eV	Scan#1
2	496	19.69872
3	496.1	17.95129
4	496.2	19.18263
5	496.3	18.03784
6	496.4	19.03867
7	496.5	18.80417
8	496.6	19.32572

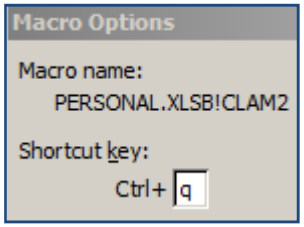
- Two-column data in the spreadsheet format are analyzed in the code.
- Worksheet is named after workbook filename.
- Syntax in A1 cell corresponds to the following.



Syntax in A1 cell	Data in column A	Data in column B
KE/eV	KE	XPS
BE/eV	BE	XPS
PE/eV	PE	XAS
GE/eV	PE	G scan
AE/eV	EE	Auger
QE/eV	mass	Q-mass
ME/eV	Position	Any

Installation of the code in Excel

- Generate **Personal Workbook Macro**
- Install **Solver** Add-in and setup its DLL
- Setup the **Shortcut key** in Macro Option



- Compile your own **database** for BE and sensitivities on UD.xlsx

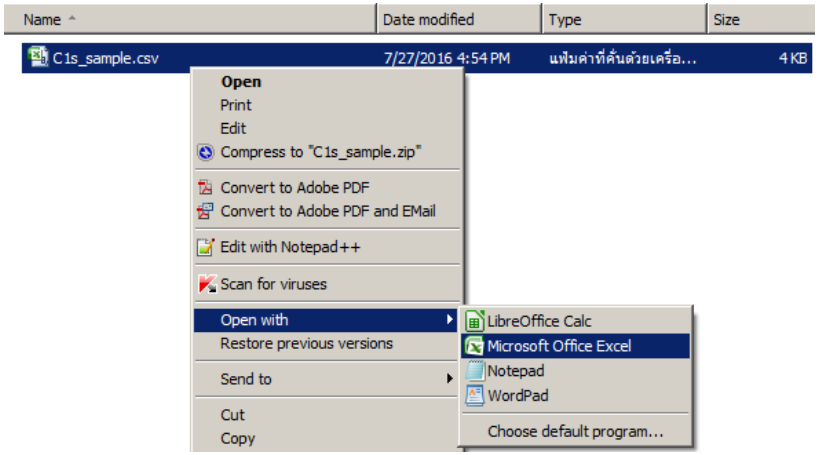
XPS worksheet

	A	B	C	D
1	Element	Orbit	BE(eV)	ASF
2	C	1s	284.6	1
3	O	1s	532	2.93

AES worksheet

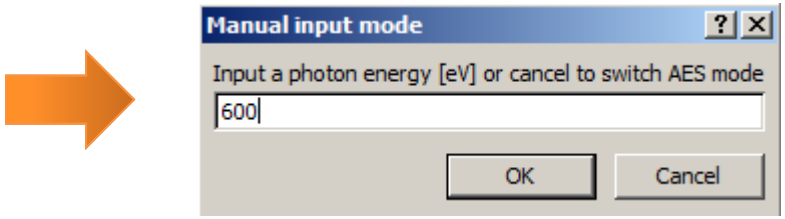
	A	B	C	D
1	Element	Auger	KE(eV)	RSF
2	C	KLL	266	0.6
3	O	KLL	506	0.96

C1s sample csv or txt

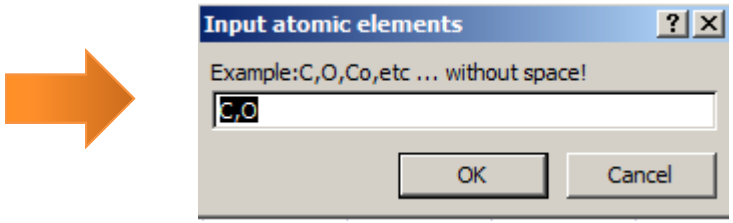


	A	B
1	KE/eV	PE: 600 eV
2	290	1709
3	290.1	1798
4	290.2	1845
5	290.3	1722
6	290.4	1729
7	290.5	1699
8	290.6	1727
9	290.7	1693
10	290.8	1647
11	290.9	1684
12	291	1659

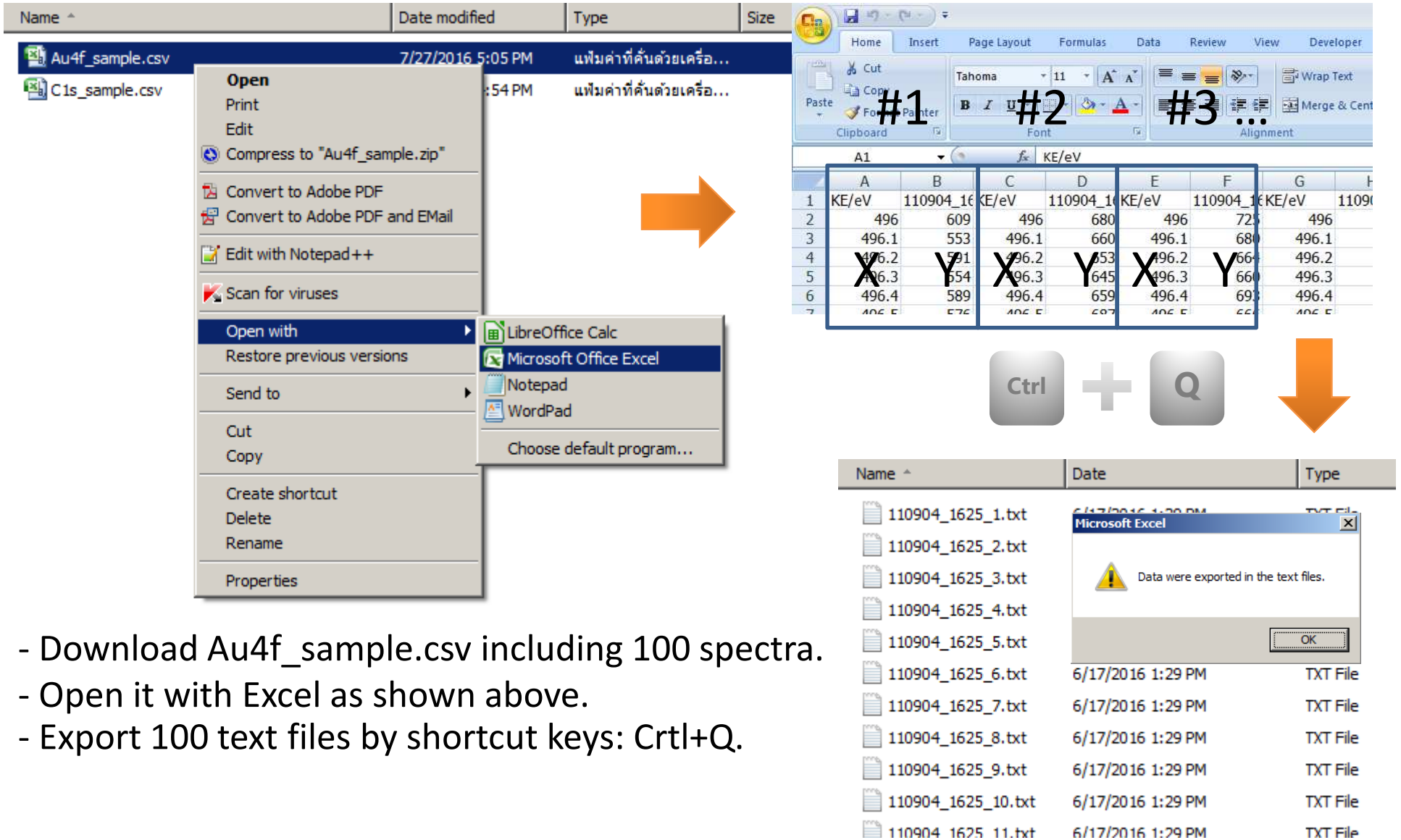
600 eV of photon energy



XPS: Carbon 1s spectrum

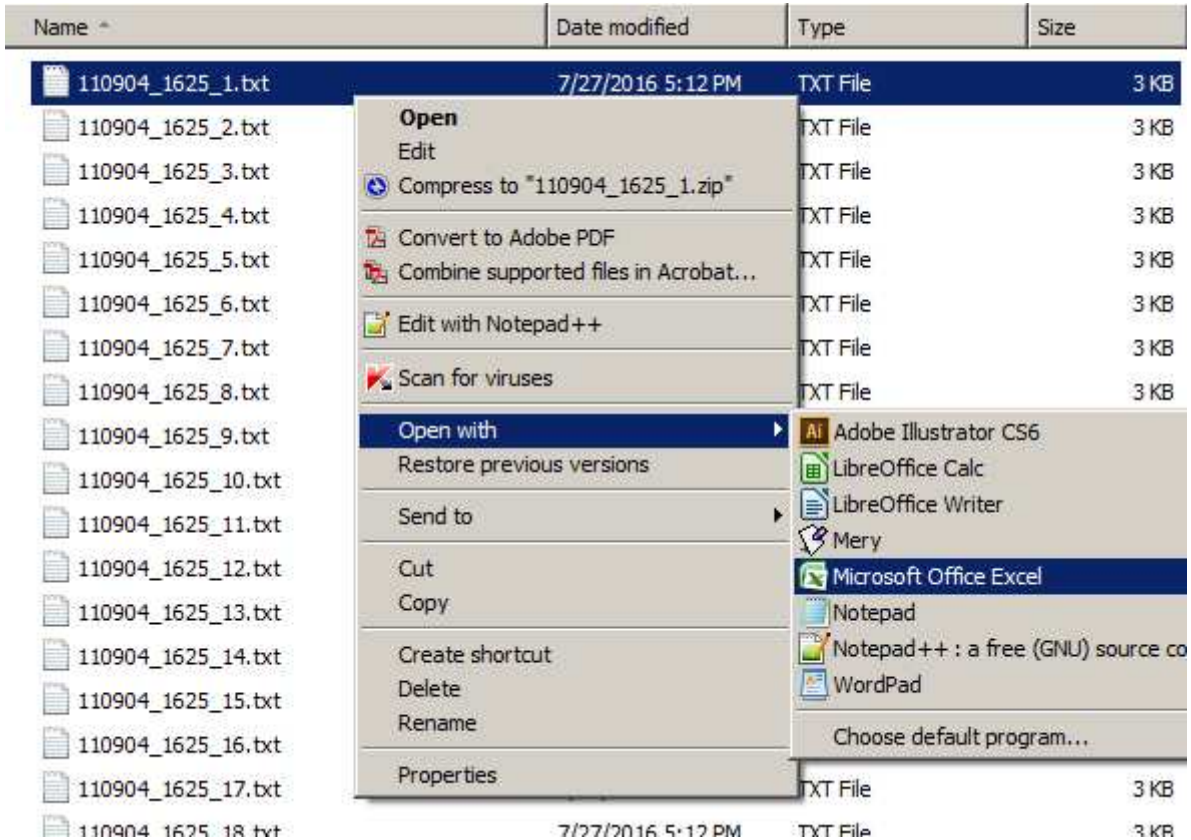


Sample file with multiple scans



- Download Au4f_sample.csv including 100 spectra.
- Open it with Excel as shown above.
- Export 100 text files by shortcut keys: Crtl+Q.

Sample file includes single data



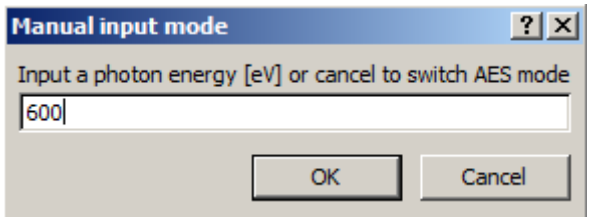
	A	B
1	KE/eV	110904_16
2	496	609
3	496.1	553
4	496.2	591
5	496.3	554
6	496.4	589
7	496.5	576
8	496.6	602
9	496.7	587
10	496.8	576
11	496.9	608

Single data to plot in Graph sheet

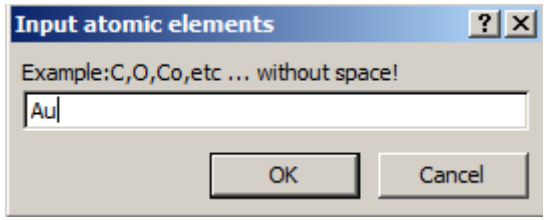
	A	B
1	KE/eV	110904_16
2	496	609
3	496.1	553
4	496.2	591
5	496.3	554
6	496.4	589
7	496.5	576
8	496.6	602
9	496.7	587
10	496.8	576
11	496.9	608

KE/eV represents a kinetic energy scale.

600 eV of photon energy



Sample: Gold metal foil



Note that Au4f sensitivity is not in database, so you have to input factors in database in a way below.

Au 4f BE and ASF
in XPS worksheet on UD.xlsx

	A	B	C	D
1	Element	Orbit	BE(eV)	ASF
2	C	1s	284.6	1
3	O	1s	532	2.93
4	Au	4f5/2	87.6	7.54
5	Au	4f7/2	84	9.58

Graph sheet

Adjustable factors

X axis

- **PE**: photon energy (eV)
- **WF**: work function (4)
- **Char**: Charging shift (0)

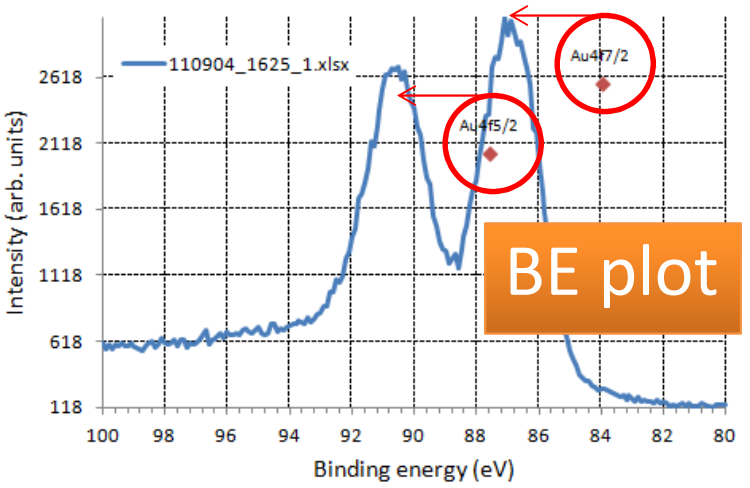
Y axis

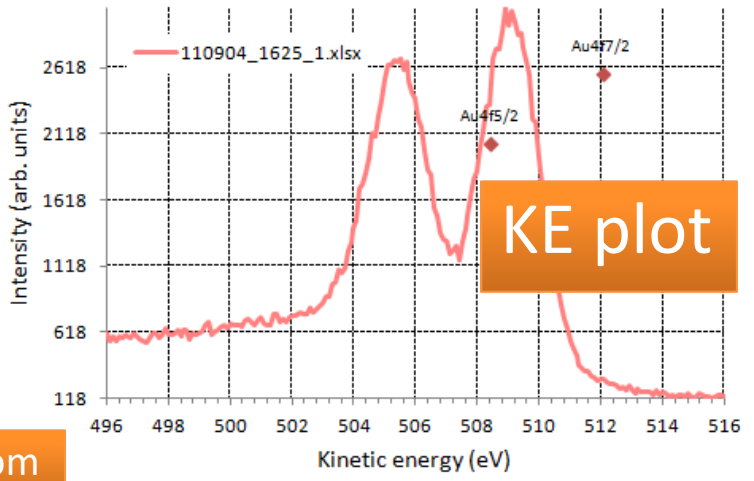
- **Offset**: constant base line (0: default)
- **Multiple**: multiple normalized factor (1)

*Change **Char** to 3, and update by*

	A	B	C
1	Grating	0	lines/mm
2	PE	600	eV
3	WF	4	eV
4	Char	0	eV
5	Start KE	496	eV
6	End KE	516	eV
7	Step KE	0.1	eV
8	# scan	1	times
9	Offset/mu	0	1
10	Ke	Be	In
11	496	100	609
12	496.1	99.9	553
13	496.2	99.8	591
14	496.3	99.7	554
15	496.4	99.6	589
16	496.5	99.5	576
17	496.6	99.4	602
18	496.7	99.3	587
19	496.8	99.2	576
20	496.9	99.1	608
	497	99	584
	497.1	98.9	566
219		110904_1625_1.xlsx	
220	Ke110904_	Be110904_	In110904_
221	496	97	609
222	496.1	96.9	553
223	496.2	96.8	591
224	496.3	96.7	554
225	496.4	96.6	589
226	496.5	96.5	576
227	496.6	96.4	602
228	496.7	96.3	587
229	496.8	96.2	576

Offset/multiple data in bottom

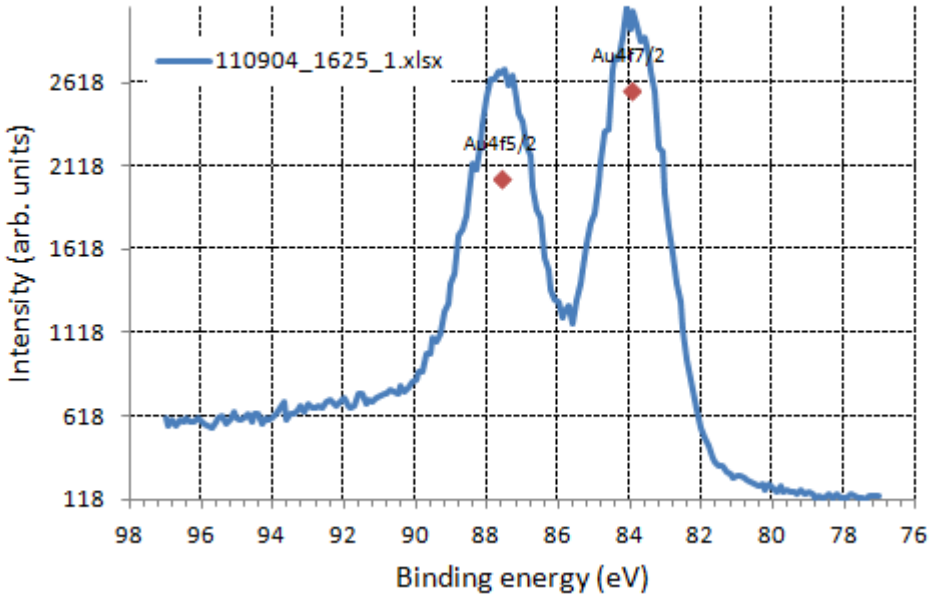




Reference spectrum

Grating	0	lines/mm
PE	600	eV
WF	4	eV
Char	3	eV
Start KE	496	eV
End KE	516	eV
Step KE	0.1	eV
# scan	1	times
Offset/mu	0	1
Ke	Be	In
496	97	609
496.1	96.9	553
496.2	96.8	591
496.3	96.7	554
496.4	96.6	589
496.5	96.5	576
496.6	96.4	602
496.7	96.3	587
496.8	96.2	576

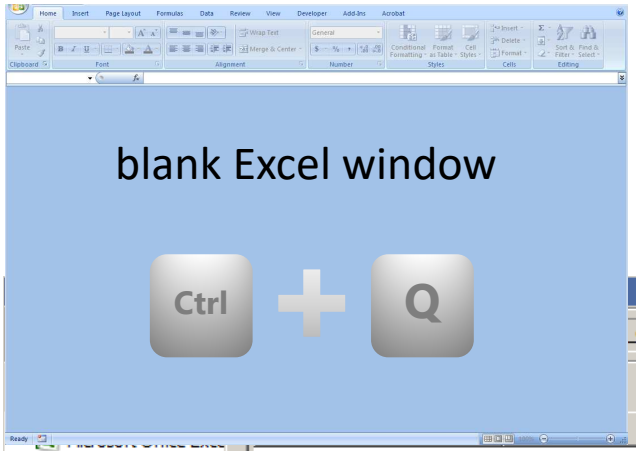
Standard peak BE should be well-known and assumed to be identical with exp.

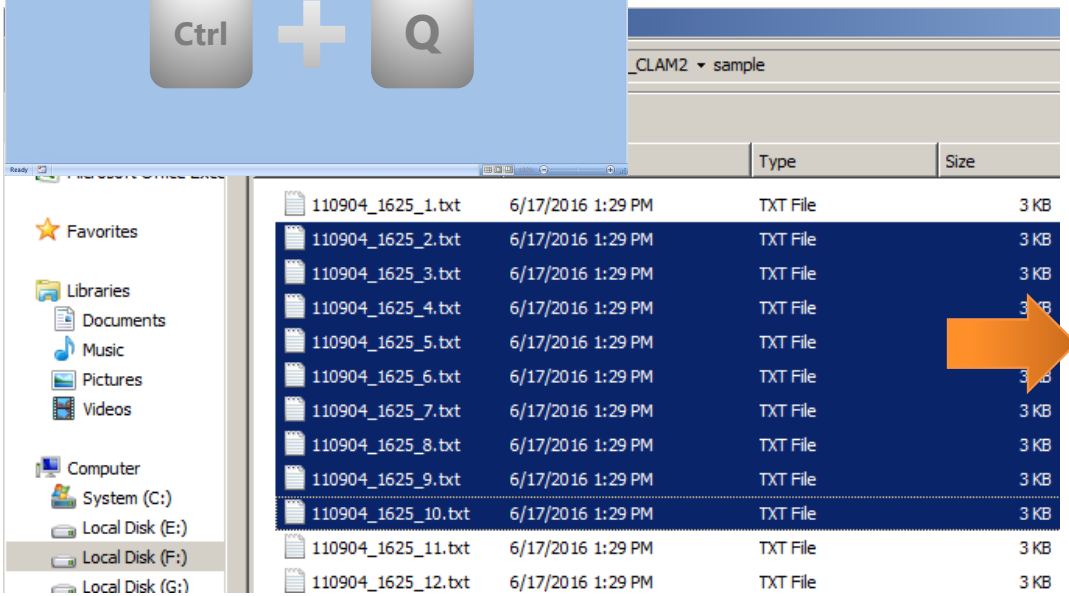


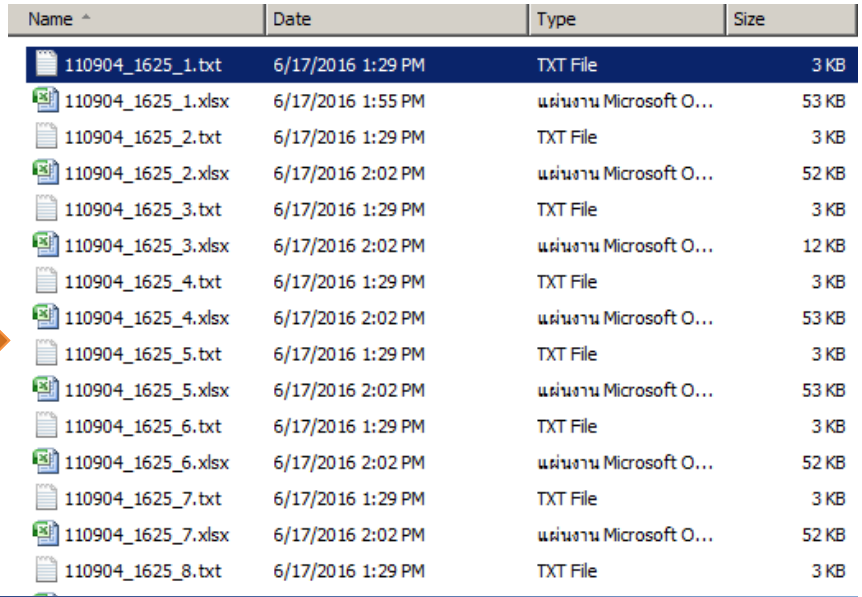
Next, apply these factors to another by "debug" in A1 cell then

	A	B	C
1	debug	0	lines/mm
2	PE	600	eV
3	WF	4	eV
4	Char	3	eV
5	Start KE	496	eV
6	End KE	516	eV
7	Step KE	0.1	eV
8	# scan	1	times
9	Offset/mu	0	1
10	Ke	Be	In

Multiple-file selection

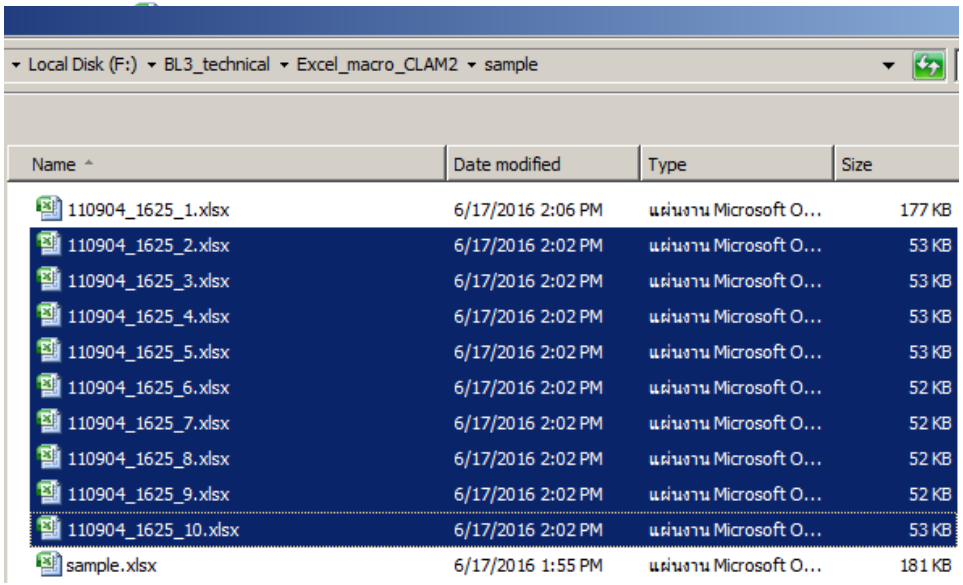






Next, compare the spectra by “comp” in D1

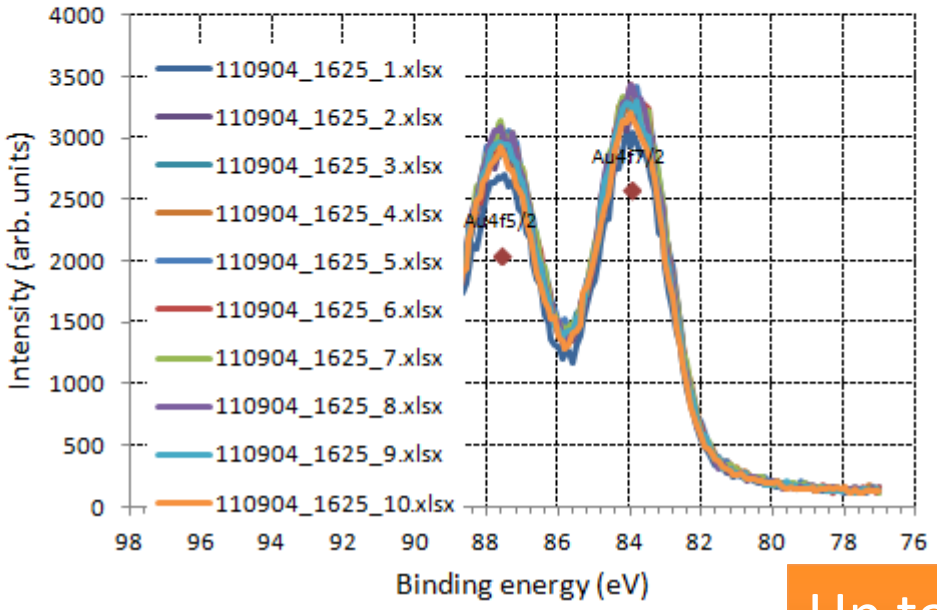
	A	B	C	D
1	Grating	0	lines/mm	comp
2	PE	600	eV	
3	WF	4	eV	
4	Char	3	eV	
5	Start KE	496	eV	
6	End KE	516	eV	
7	Step KE	0.1	eV	
8	# scan	1	times	
9	Offset/mu	0	1	
10	Ke	Be	In	
11	496	97	609	
12	496.1	96.9	553	
13	496.2	96.8	591	
14	496.3	96.7	554	
15	496.4	96.6	589	
16	496.5	96.5	576	
17	496.6	96.4	602	
18	496.7	96.3	587	

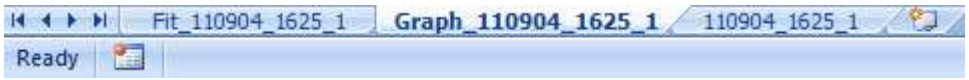


"comp" in D4 cell 

Compared spectra

Grating	0	lines/mm	comp	110904_1625_2.xlsx		110904_1625_3.xlsx		1109
PE	600	eV	PE	600	eV	PE	600	eV	PE	
WF	4	eV	WF	4	eV	WF	4	eV	WF	
Char	3	eV	Char	3	eV	Char	3	eV	Char	
Start KE	496	eV	Start KE	496	eV	Start KE	496	eV	Start KE	
End KE	516	eV	End KE	516	eV	End KE	516	eV	End KE	
Step KE	0.1	eV	Step KE	0.1	eV	Step KE	0.1	eV	Step KE	
# scan	1	times	# scan	1	times	# scan	1	times	# scan	
Offset/mu	0	1	Offset/mu	0	1	Offset/mu	0	1	Offset/mu	
Ke	Be	In	Ke	Be	In	Ke	Be	In	Ke	Be
496	97	609	496	97	680	496	97	725	496	
496.1	96.9	553	496							
496.2	96.8	591	496							
496.3	96.7	554	496							
496.4	96.6	589	496							
496.5	96.5	576	496							
496.6	96.4	602	496							
496.7	96.3	587	496							
496.8	96.2	576	496							
496.9	96.1	608	496							
497	96	584	4							
497.1	95.9	566	49							
497.2	95.8	555	49							
497.3	95.7	543	49							
497.4	95.6	576	49							
497.5	95.5	606	49							
497.6	95.4	614	49							
497.7	95.3	575	49							





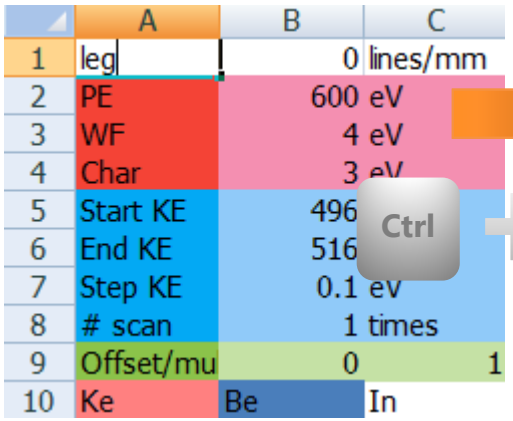
Up to 100 spectra for BE&KE plots

Analysis on spectra compared

- Automatically scaled spectra for comparison
  - “auto” in A1 cell to scale at the both ends
  - “auto[x1:x2,x3:x4]” in A1 cell to scale in the ranges of (x1, x2) for offset (0) and (x3, x4) for multiple (1).
  - “auto{284.6}” in A1 cell to shift the maximum intensity to 284.6 eV in BE scale.
  - “auto’-7.8’” in A1 cell to set all char factor to be -7.8 eV.
- Annotate legends in each plot
  - “leg” in A1 cell to generate Sample sheet
  - Describe sample or spectrum name in the sheet
  - “leg” in A1 cell to run the code again.
- Normalize spectra with ref. spectrum by “norm” in A1 cell.
  - Second set of data will be selected for ref. and third set to be normalized data.
  - Norm sheet appears from the data normalized.

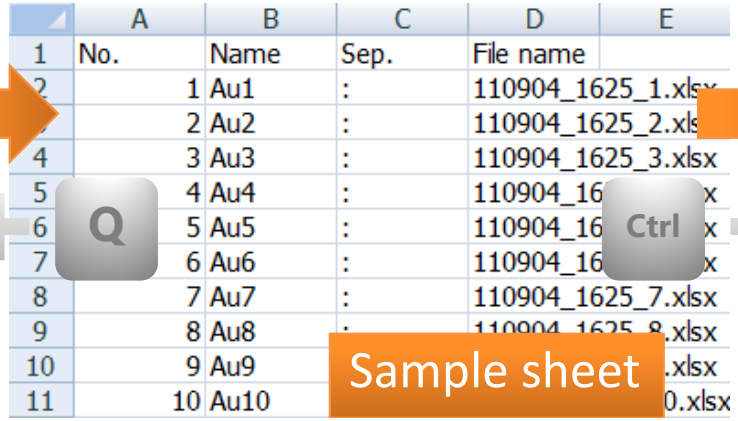
Every single step needs

Ctrl + Q



	A	B	C
1	leg	0	lines/mm
2	PE	600	eV
3	WF	4	eV
4	Char	3	eV
5	Start KE	496	
6	End KE	516	
7	Step KE	0.1	eV
8	# scan	1	times
9	Offset/mu	0	1
10	Ke	Be	In

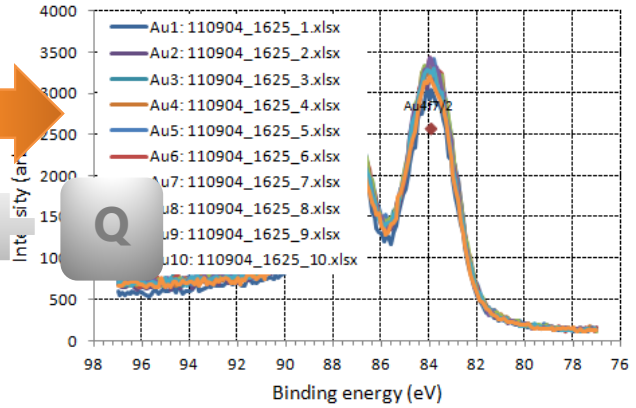
Ctrl + Q



	A	B	C	D	E
1	No.	Name	Sep.	File name	
2	1	Au1	:	110904_1625_1.xlsx	
3	2	Au2	:	110904_1625_2.xlsx	
4	3	Au3	:	110904_1625_3.xlsx	
5	4	Au4	:	110904_16	x
6	5	Au5	:	110904_16	x
7	6	Au6	:	110904_16	x
8	7	Au7	:	110904_1625_7.xlsx	
9	8	Au8	:	110904_1625_8.xlsx	
10	9	Au9	:	110904_1625_9.xlsx	
11	10	Au10	:	110904_1625_10.xlsx	

Sample sheet

Ctrl + Q



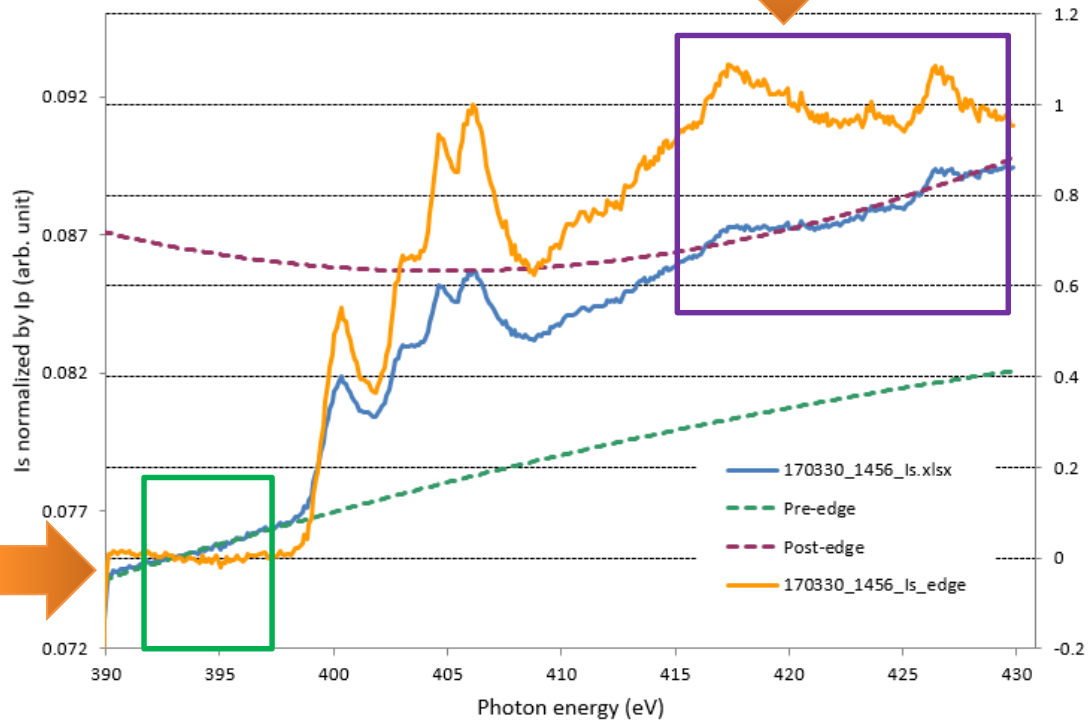
Edge correction in NEXAFS

	1	2	3	4	5	6	7	8	9
1	edge	1200	lines/mm		Pre edge	Post edge		170330_1456_Is_edge	
2	PE shifts	-0.17	eV	Start, eV	392	415	PE shifts	0	eV
3	Smoothin	4	points	End, eV	397	429			
4					Polynominal coeff				
5	Start PE	390	eV	a0	0.078983	0.085857	Start PE	389.83	eV
6	End PE	430	eV	a1	0.003787	0.001334	End PE	429.83	eV
7	Step PE	0.1	eV	a2	-0.00071	0.002589	Step PE	0.1	eV
8	# scan	1	times	a3	0	0			
9	Offset/mu	0	1	chi^2	7.03E-08	9.53E-07	Offset/mu	0	1
10	PE	Ab	De	PE	Pre-edge	Post-edge	Pe	Ab	De

New *spline edge correction*
A1 cells: “edge”
New *Linear combination*
A1 cells: “lcmb”
After two references added.

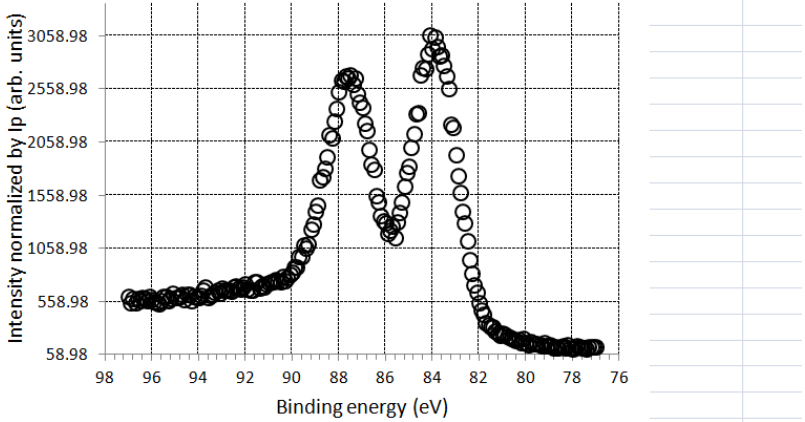
Post-edge region to be 1

Pre-edge regions to be 0



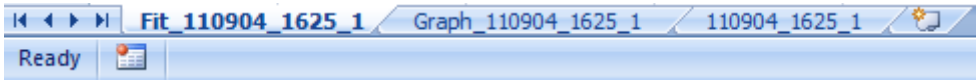
Fit sheet

	A	B
1	Shirley	BG
2	Tolerance	0.000001
3	Initial A	0.001
4	Final A	
5	Iteration	
6		
7		
8		
9		
10		
11	Solve BGS	
12	Peak fit	
13	# peaks	
14	Solve LSM	
15	Fit range	
16	Start / eV	77
17	End / eV	97
18	Factors for N.Area	
19	CAE	23.5
20	Grating	0
21	IMFP	0.6
22	a	180.254
23	b	0.348
24	theta	45
25		
26		
27		
28		
29		
30	BE / eV	In
31	97	609
32	96.9	553
33	96.8	591



Ctrl + Q

Data appear here from the latest updated Graph sheet.



Switch the worksheet

Note that offset/multiple factors should be aligned for all spectra in Graph sheet to evaluate the peak area in Fit sheet.

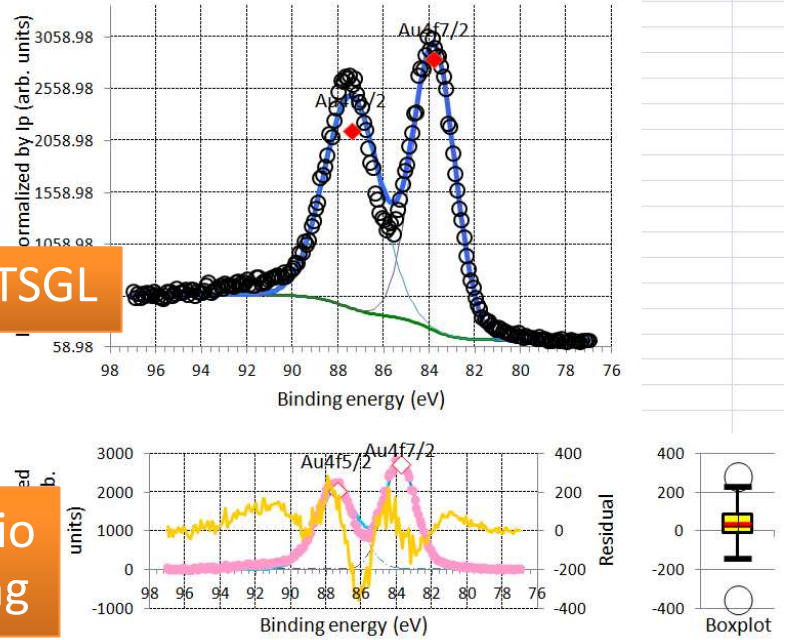
Fitting functions and parameters

Shirley, **T**ougaard, **P**olynomial, **P**oly **S**hirley, **P**oly **T**ougaard, **V**ictoreen, **A**rctan

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Shirley	BG		Name	Au4f7/2	Au5/2											
2	Tolerance	0.000001		BE	83.79984	87.39984											
3	Initial A	0.001		KE	509.2002	505.6002											
4	Final A	0.00344		FWHM1	2.178228	2.847956											
5	Iteration	10		FWHM2													
6				Amplitude	2728.653	2046.49											
7				Shape	Gauss	Gauss											
8				Option a													
9				Option b													
10				Option c													
11	Solve BGS	0.533817		Form	G	G											
12	Peak fit			beta	0.7075	0.7075											
13	# peaks	2		Amp+BG	2846.653	2164.49											
14	Solve LSM	11.90548	χ^{2*}	RSF	99.15739	78.04245											
15	Fit range			P. Area	6338.166	6215.195											
16	Start / eV	77		S. Area	63.92026	79.63864											
17	End / eV	97		N. Area	71.27218	89.17103											
18	Factors for N.Area			Asym													
19	CAE	23.5		Amp. rat.	(4;	3)											
20	Grating	0		BE diff.	[	3.6]											
21	IMFP	0.6		T.I. Area	6339.774	6216.771											
22	a	180.254		S.I. Area	63.93647	79.65884											
23	b	0.348		N.I. Area	71.29025	89.19364											
24	theta	45		Corr. RSF	88.92904	69.69971											
25																	
26																	
27																	
28																	
29																	
30	BE / eV	In	BG	In-BG	Au4f7/2	Au5/2	SUM fits	Least fits	Residual								
31	97	609	584.9897	24.01026	2.49E-41	4.84E-11	4.84E-11	0.985475	24.01026								
32	96.9	553	584.9686	-31.96863	1.15E-40	9.27E-11	9.27E-11	1.747091	-31.96863								

G, L, GL, SGL, TSGL

Amplitude ratio
Energy splitting



Update results by setup **constraints with bold font style**, various BGs or Forms

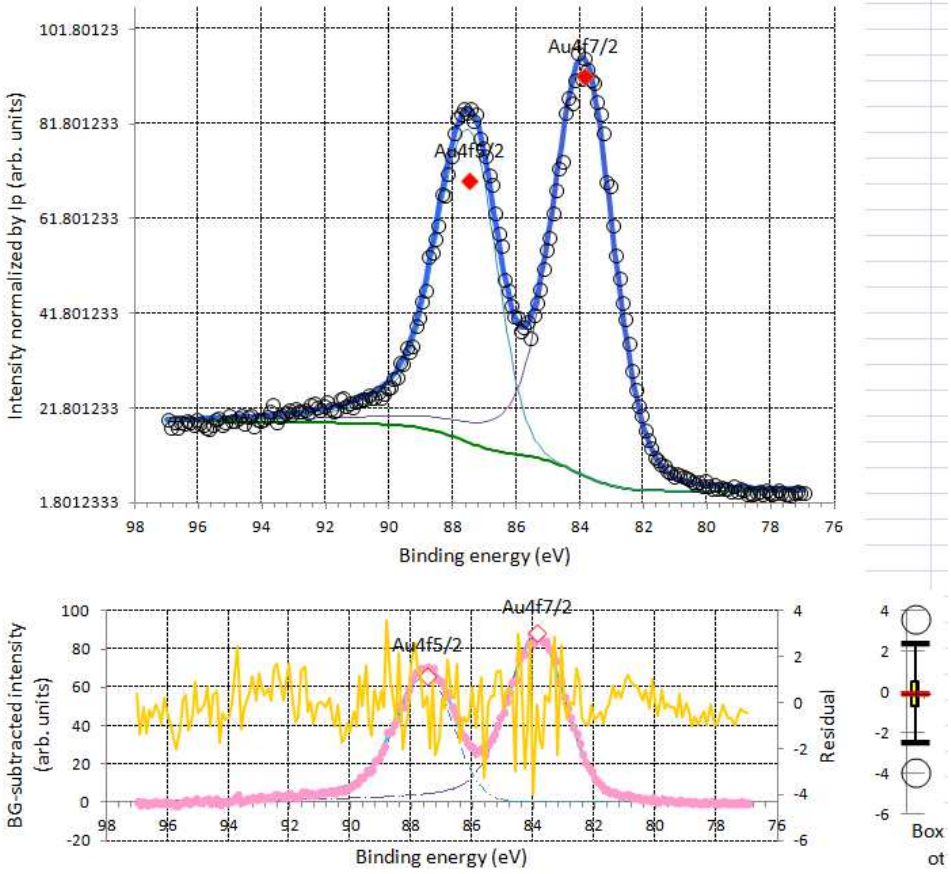
Ctrl + Q

FWHM ranges can also be setup.

Peak shape: Tailed pseudo-Voigt

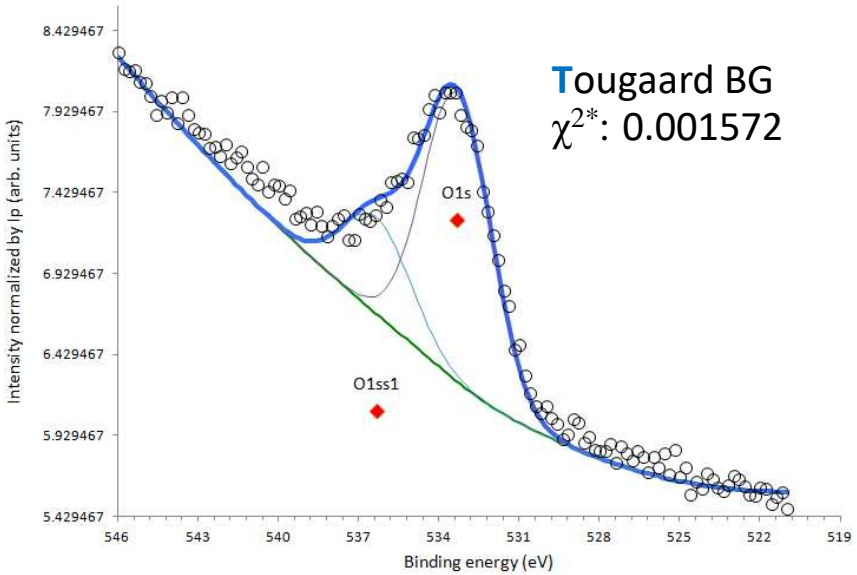
	A	B	C	D	E	F
1	Shirley	BG		Name	Au4f7/2	Au4f5/2
2	Tolerance	0.000001		BE	83.89177	87.49177
3	Initial A	0.001		KE	509.1082	505.5082
4	Final A	0.0036		FWHM1	2.192026	2.036631
5	Iteration	3		FWHM2		
6				Amplitude	88.24273	66.18205
7				Shape	0.207135	0.001
8				Option a	0.0927	0.442394
9				Option b	20.46306	11.55928
10				Option c		
11	Solve BGS	0.01586		Form	TSGL	TSGL
12	Peak fit			beta	0.7075	0.7075
13	# peaks	2		Amp+BG	91.91117	69.85049
14	Solve LSM	0.045204	χ^{2*}	RSF	99.15739	78.04245
15	Fit range			P. Area	226.4484	143.8036
16	Start / eV	77		S. Area	2.283727	1.842633
17	End / eV	97		N. Area	2.546665	2.063409
18	Factors for N.Area			Asym		
19	CAE	23.5		Amp. rat.	(4;	3)
20	Grating	0		BE diff.	[	3.6]
21	IMFP	0.6		T.I. Area	240.0941	171.4606
22	a	180.254		S.I. Area	2.421343	2.197018
23	b	0.348		N.I. Area	2.700126	2.460255
24	theta	45		Corr. RSF	88.91957	69.69223

	A	B	C	D	E	F	G	H	I
30	BE / eV	In	BG	In-BG	Au4f7/2	Au4f5/2	SUM fits	Least fits	Residual
31	97	19.69872	18.94799	0.750731	0.271886	0.111915	0.383802	0.006965	0.36693
32	96.9	17.95129	18.94713	-0.99584	0.278361	0.118642	0.397003	0.100289	-1.39284
33	96.8	19.18263	18.94387	0.238762	0.285022	0.125775	0.410797	0.001529	-0.17204
34	96.7	18.03784	18.94352	-0.90568	0.291876	0.133338	0.425214	0.091451	-1.3309
35	96.6	19.03867	18.94303	0.095641	0.298928	0.141357	0.440284	0.006128	-0.34464
36	96.5	18.80417	18.94164	-0.13747	0.306184	0.149859	0.456043	0.01816	-0.59352

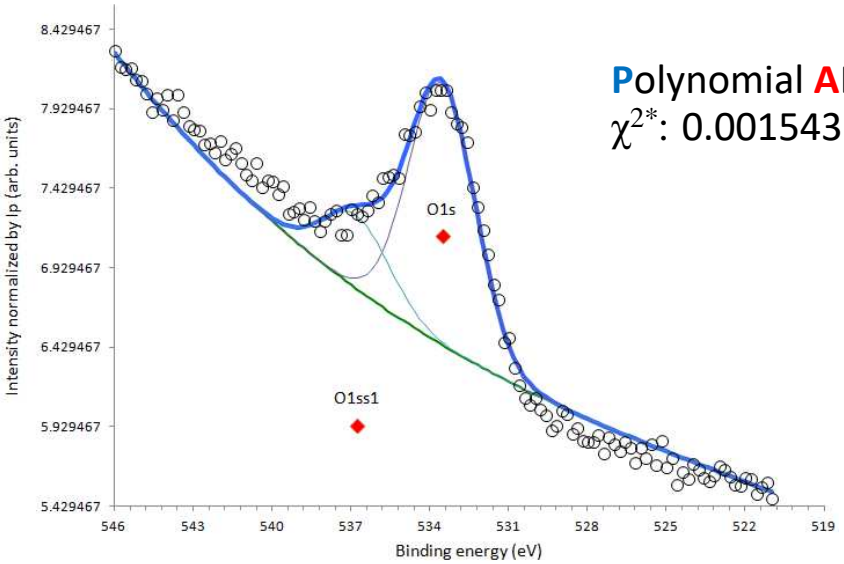


Shirley's BG, Tailed Voigt, Doublet 4f (4:3), ΔSO Au4f: 3.6 eV are used for above fitting.
User-defined peak and BG functions can be easily implemented in your Visual Basic code.

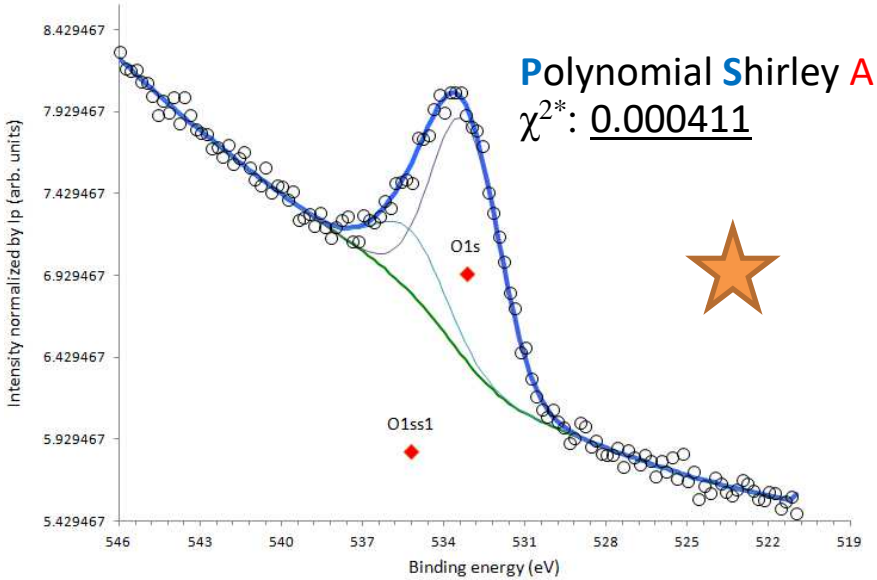
Polynomial (Shirley or Tougaard) Active-BGs



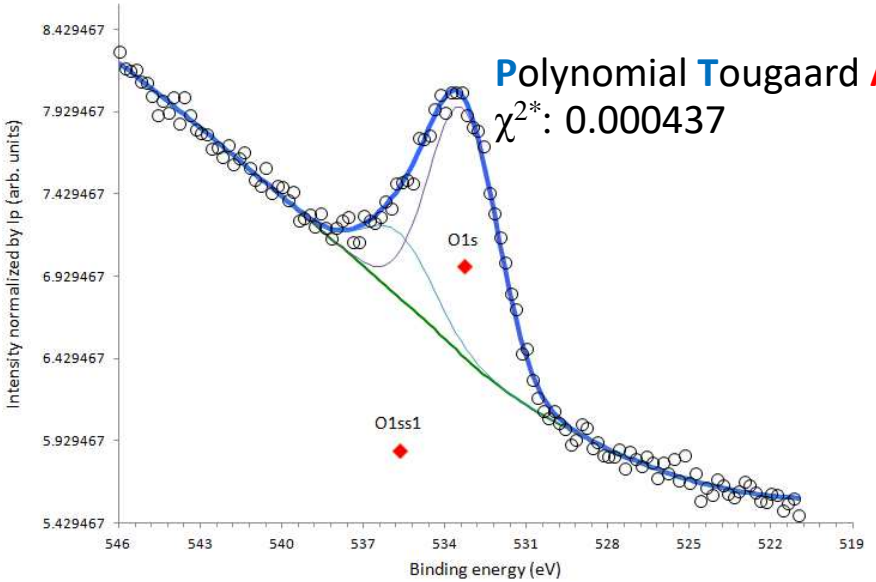
Tougaard BG
χ^{2*}: 0.001572



Polynomial ABG
χ^{2*}: 0.001543



Polynomial Shirley ABG
χ^{2*}: 0.000411



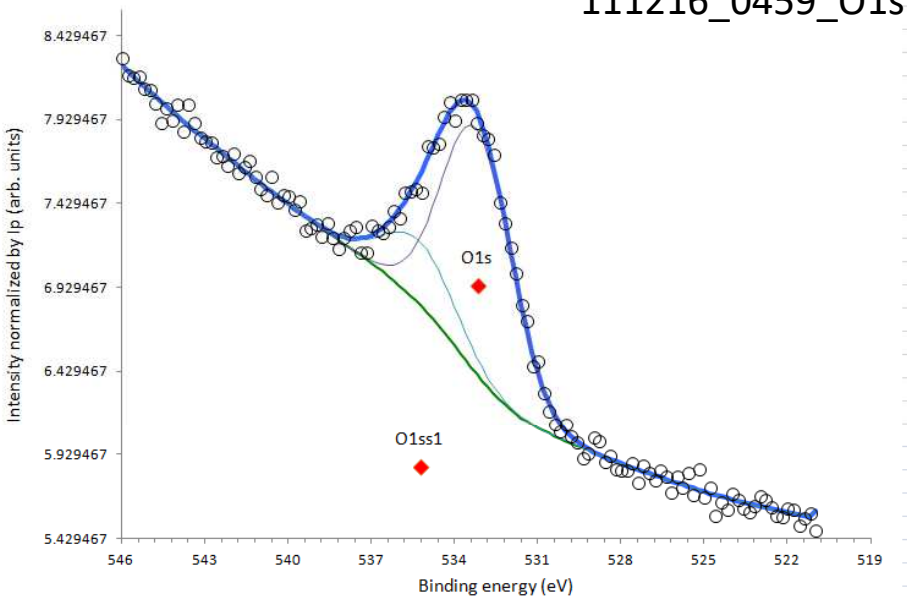
Polynomial Tougaard ABG
χ^{2*}: 0.000437

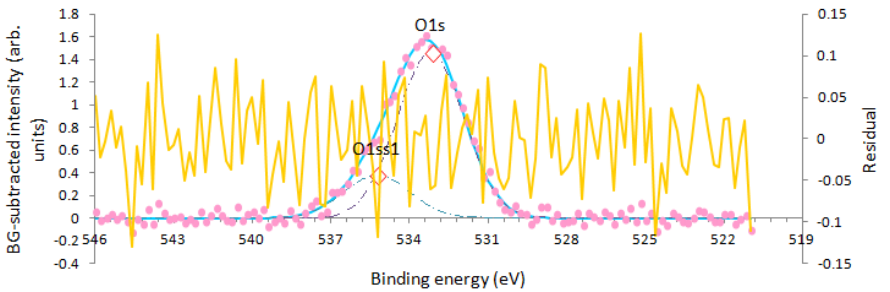
Poly Shirley ABG

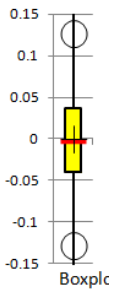
	A	B	C	D	E	F
1	Polynomin	Shirley	ABG	Name	O1s	O1ss1
2	Tolerance	0.000001		BE	533.1928	535.2478
3	Initial A	0.001		KE	62.80724	60.75223
4	Final A	0.236075		FWHM1	3	3
5	Iteration	1		FWHM2		
6	Ratio S:P	0.068965		Amplitude	1.461219	0.377278
7	0th poly	6.299347		Shape	Gauss	Gauss
8	1st poly	-1.1533		Option a		
9	2nd poly	0.414044		Option b		
10	3rd poly	-0.00799		Option c		
11	Solve BGS	0.00036		Form	G	G
12	Peak fit			beta	2	2
13	# peaks	2		Amp+BG	6.947018	5.863077
14	Solve LSM	0.000411	χ^{2*}	RSF	30.13401	30.13401
15	Fit range			P. Area	4.674643	1.206965
16	Start / eV	521		S. Area	0.155128	0.040053
17	End / eV	546		N. Area	0.461899	0.121174
18	Factors for N.Area			Asym		
19	CAE	100		Amp. rat.		
20	Grating	2		BE diff.		
21	IMFP	0.6		T.I. Area	4.675828	1.207271
22	a	1.35		S.I. Area	0.155168	0.040063
23	b	0.35		N.I. Area	0.462016	0.121205
24	theta	90		Corr. RSF	10.12048	9.960556

	A	B	C	D	E	F	G	H	I
30	BE / eV	In	BG	In-BG	O1s	O1ss1	SUM fits	Least fits	Residual
31	546	8.30239	8.250327	0.052063	2.04E-22	1.49E-16	1.49E-16	0.000329	0.052063
32	545.8	8.197874	8.220507	-0.02263	9.7E-22	5.5E-16	5.5E-16	6.23E-05	-0.02263
33	545.6	8.187272	8.190389	-0.00312	4.5E-21	1.98E-15	1.98E-15	1.19E-06	-0.00312
34	545.4	8.195189	8.160879	0.03431	2.04E-20	6.97E-15	6.97E-15	0.000144	0.03431
35	545.2	8.121771	8.131507	-0.00974	9E-20	2.39E-14	2.39E-14	1.17E-05	-0.00974
36	545	8.116025	8.101951	0.014074	3.88E-19	8.02E-14	8.02E-14	2.44E-05	0.014074
37	544.8	8.033022	8.07112	-0.0381	1.63E-18	2.62E-13	2.62E-13	0.00018	-0.0381
38	544.6	7.913207	8.042458	-0.12925	6.7E-18	8.37E-13	8.37E-13	0.002077	-0.12925
39	544.4	8.004564	8.013261	-0.0087	2.69E-17	2.6E-12	2.6E-12	9.44E-06	-0.0087
40	544.2	7.929674	7.984054	-0.05438	1.05E-16	7.91E-12	7.91E-12	0.00037	-0.05438
41	544	8.022887	7.955162	0.067725	4E-16	2.34E-11	2.34E-11	0.000577	0.067725

111216_0459_O1s.xlsx







3-eV FWHM Gaussian fit

Lists of fitting functions

Peak shapes (total 5 forms)

Code (form)	Shape	Option a	Option b
G (0)	Gauss		
L (1)	Lorentz		
GL (0 < shape < 1)	G + L with the same FWHM1		
SGL (0 < shape < 1)	G (FWHM1) + L (FWHM2)		
TSGL	Exponential blend GL (FWHM1)	Tail scale	Tail length at half max

Backgrounds (total 9 BGs)

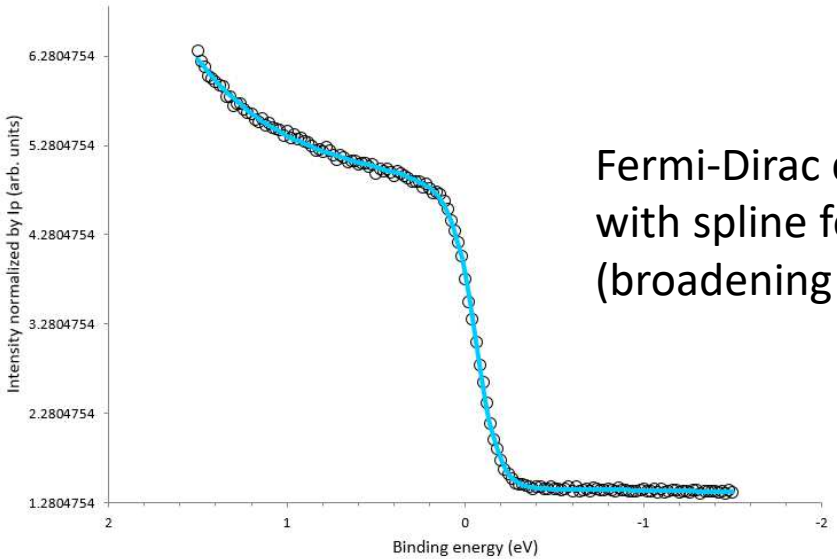
BG (A1)	BG (B1)	BG (C1)	Technique	Optimization
Shirley	BG/ABG		XPS	Static/Active
Tougaard	BG		XPS	Static
Polynomial	BG/ABG		XPS/XAS	Static/Active
Polynomial	Shirley	ABG	XPS	Active
Polynomial	Tougaard	ABG	XPS	Active
Victoreen	BG		XAS	Static
ArcTangent	BG		XAS	Active

Sigmoid (convoluted) fitting

	A	B	C	D	E
1	Sigmoid			Name	Inf_1
2	Int BG/DO	1.433601	3.172378	BE	-0.06522
3	Slope BG/	0.004339	1.194389	KE	35.56522
4	Poly2 BG/	-0.00508	-1.14319	Temp	741.598
5	Poly3 BG/	0.006218	0.663992	Width(FD	0.28056
6				Width(GC	0
7				Total	0.28056
8	Norm (FD	0.0001	0	Norm (GC	0.860253
9					
10	Solve FD	0.000647			
11	Solve GC				
12	Peak fit				
13	BE min	-1.5			
14	BE max	1.5			
15	Fit range				
16	Start / eV	-1.5			
17	End / eV	1.5			
18	Factors for N.Area				
19	CAE	10			
20	Grating	1			
21	IMFP	0.6			
22	a	1.35			
23	b	0.35			
24	theta	90			
25	Figure of merit				

EF range

Fit range



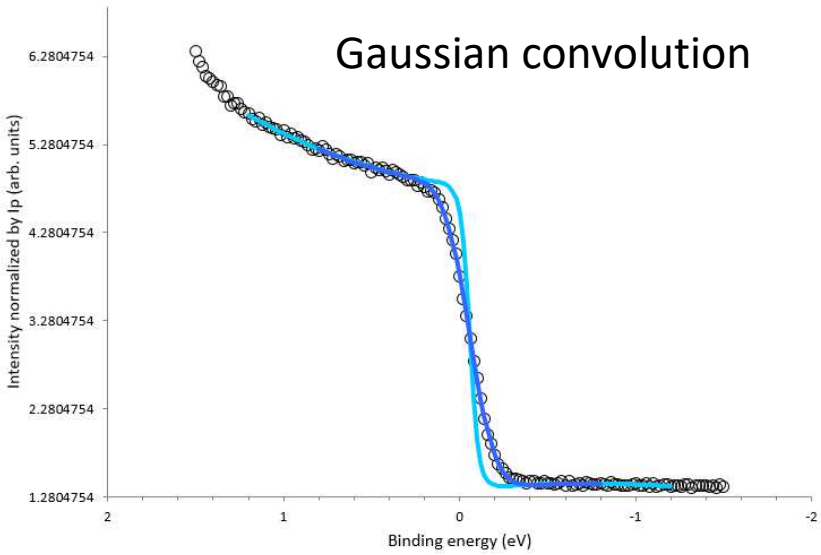
Fermi-Dirac distribution
with spline for the Fermi edge
(broadening only from temp)

Constraint temperature at 300 K, and polynomial parameters as well prior to convolution. Sample temp. leads to ΔE=113 meV, and instrumental resolution (BL & analyzer) to 243 meV. Total resolution becomes ΔE=268 meV.

Secondary electron cutoff can be analyzed in the same way.

	A	B	C	D	E
1	Sigmoid	nvolute	Fit	Name	Inf_1
2	Int BG/DO	1.376123	3.441427	BE	-0.05806
3	Slope BG/	-0.16666	0.324522	KE	35.55806
4	Poly2 BG/	-0.12576	0.503831	Temp	300
5	Poly3 BG/	0	0	Width(FD	0.113495
6				Width(GC	0.243064
7				Total	0.268256
8	Norm (FD	0.0001	0	Norm (GC	0.384627
9					
10	Solve FD	0.038662			
11	Solve GC	0.000621			
12	Peak fit				
13	BE min	-1.2			
14	BE max	1.2			
15	Fit range				
16	Start / eV	-1.2			
17	End / eV	1.2			
18	Factors for N.Area				
19	CAE	10			
20	Grating	1			
21	IMFP	0.6			
22	a	1.35			
23	b	0.35			
24	theta	90			
25	Figure of merit				

Gaussian convolution



ULVAC-PHI

Multipak csv data analysis

Open Multipak-exported csv file with Excel, and type “phi” on B1 cell.

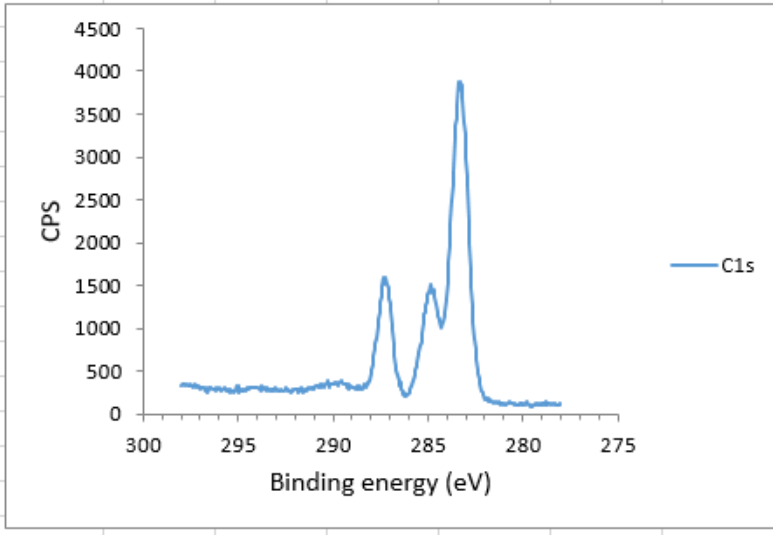
PET.csv	2/19/2016 2:40 PM	Microsoft Excel C...	8 KB
PET.SPE	1/7/2015 4:45 PM	SPE File	7 KB

Run the macro, then new workbook appears with chart of spectrum in the csv file.

	A	B	C	D
1	Area4	phi		
2	PET			
3	C1s			
4	1			
5	298	324.2826		
6	297.95	352.4358		
7	297.9	342.0087		
8	297.85	342.0087		
9	297.8	326.368		
10	297.75	356.6066		
11	297.7	344.0941		
12	297.65	332.6243		
13	297.6	332.6243		
14	297.55	329.4962		
15	297.5	339.9232		
16	297.45	328.4535		

Ctrl + Q

	A	B	C	D	E	F	G	H	I
1	Area4	Analyzed							
2	PET								
3	C1s								
4	1								
5	298	324.2826							
6	297.95	352.4358							
7	297.9	342.0087							
8	297.85	342.0087							
9	297.8	326.368							
10	297.75	356.6066							
11	297.7	344.0941							
12	297.65	332.6243							
13	297.6	332.6243							
14	297.55	329.4962							
15	297.5	339.9232							
16	297.45	328.4535							



Open text file with Excel.

PET.csv	2/19/2016 2:40 PM	Microsoft Excel C...	8 KB
PET.SPE	1/7/2015 4:45 PM	SPE File	7 KB
PET.xlsx	5/8/2019 2:28 PM	Microsoft Excel W...	25 KB
PET_C1s.txt	5/8/2019 2:28 PM	TXT File	7 KB

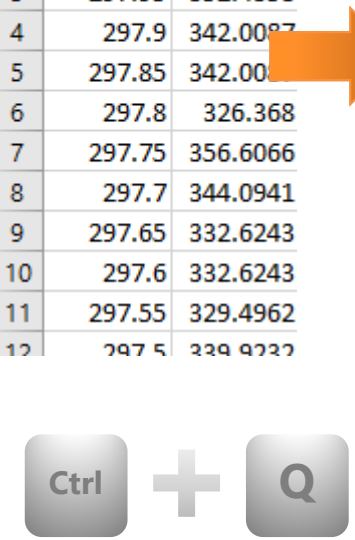
Open Excel macro-exported txt file with Excel.

PET.csv	2/19/2016 2:40 PM	Microsoft Excel C...	8 KB
PET.SPE	1/7/2015 4:45 PM	SPE File	7 KB
PET.xlsx	5/8/2019 2:28 PM	Microsoft Excel W...	25 KB
PET_C1s.txt	5/8/2019 2:28 PM	TXT File	7 KB

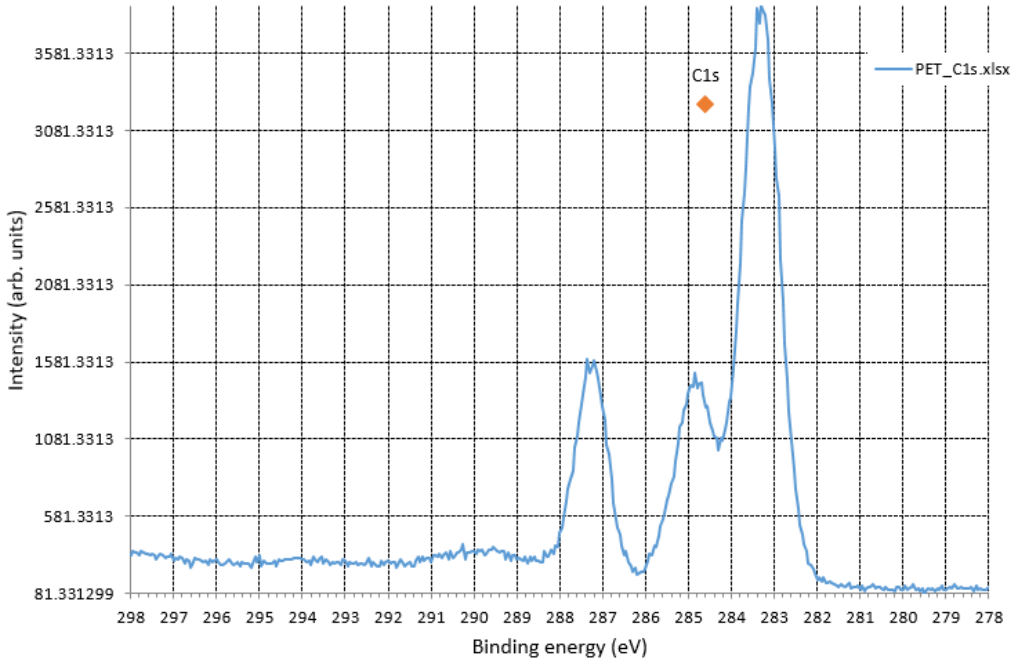
continued

Run the macro.

	A	B
1	BE/eV	AlKa
2	298	324.2826
3	297.95	352.4358
4	297.9	342.0087
5	297.85	342.00
6	297.8	326.368
7	297.75	356.6066
8	297.7	344.0941
9	297.65	332.6243
10	297.6	332.6243
11	297.55	329.4962
12	297.5	339.9232



	A	B	C
1	Grating	0	lines/mm
2	PE	1486.6	eV
3	WF	4	eV
4	Char	0	eV
5	Start BE	298	eV
6	End BE	278	eV
7	Step BE	-0.05	eV
8	# scan	1	times
9	Offset/mu	0	1
10	Ek	Be	In
11	1184.6	298	324.2826
12	1184.65	297.95	352.4358
13	1184.7	297.9	342.0087
14	1184.75	297.85	342.0087
15	1184.8	297.8	326.368
16	1184.85	297.75	356.6066
17	1184.9	297.7	344.0941
18	1184.95	297.65	332.6243
19	1185	297.6	332.6243
20	1185.05	297.55	329.4962
21	1185.1	297.5	339.9232
22	1185.15	297.45	328.4535
23	1185.2	297.4	304.4711
24	1185.25	297.35	326.368
25	1185.3	297.3	338.8806
26	1185.35	297.25	328.4535



PET.csv	2/19/2016 2:40 PM	Microsoft Excel C...	8 KB
PET.SPE	1/7/2015 4:45 PM	SPE File	7 KB
PET.xlsx	5/8/2019 2:28 PM	Microsoft Excel W...	25 KB
PET_C1s.txt	5/8/2019 2:28 PM	TXT File	7 KB
PET_C1s.xlsx	5/8/2019 2:36 PM	Microsoft Excel W...	91 KB

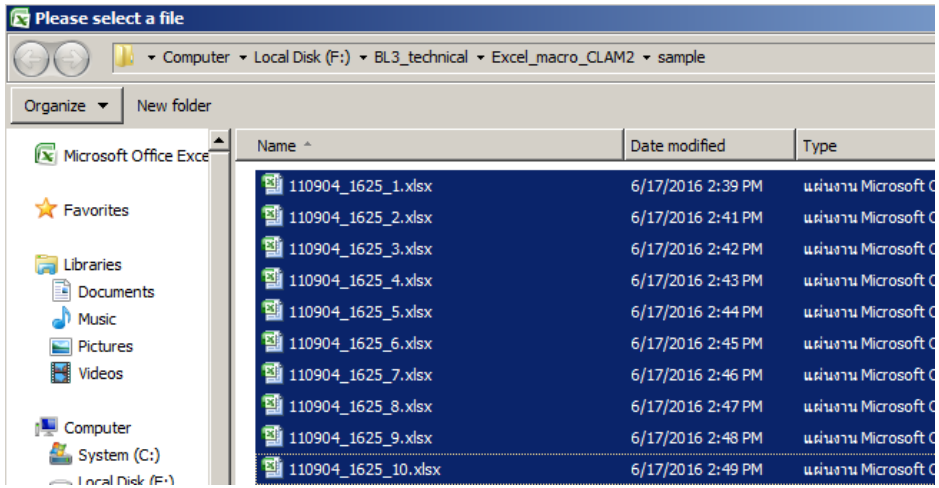
Multiple data-fit

	A	B	C	D	E	F
1	Shirley	BG		debug	Au4f7/2	Au4f5/2
2	Tolerance	0.000001		BE	83.89131	87.49132
3	Initial A	0.001		KE	509.1087	505.5087
4	Final A	0.00344		FWHM1	2.196802	2.052602
5	Iteration	6		FWHM2		

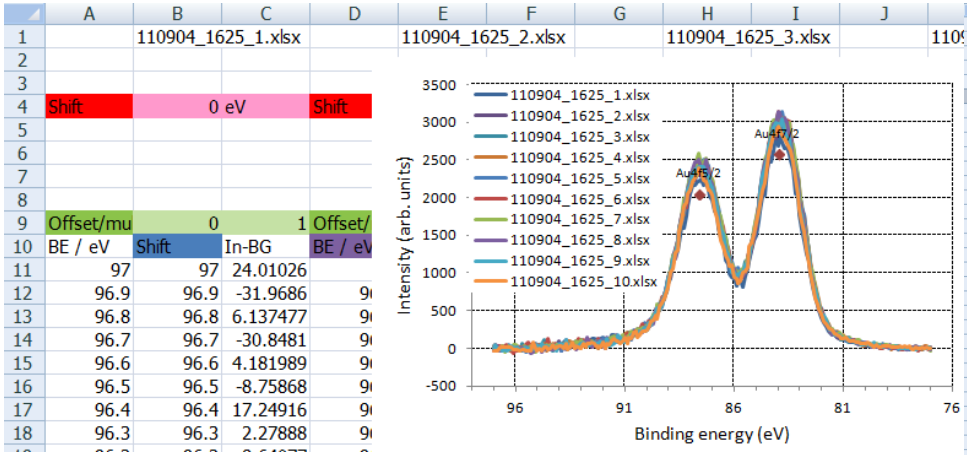
"debug"/"debuga" in D1 cell
- debug: apply the original fit parameters
- debuga: apply those used just before

Once fitting process above done, "ana" in D1 cell to compare those fitted xlsx files.

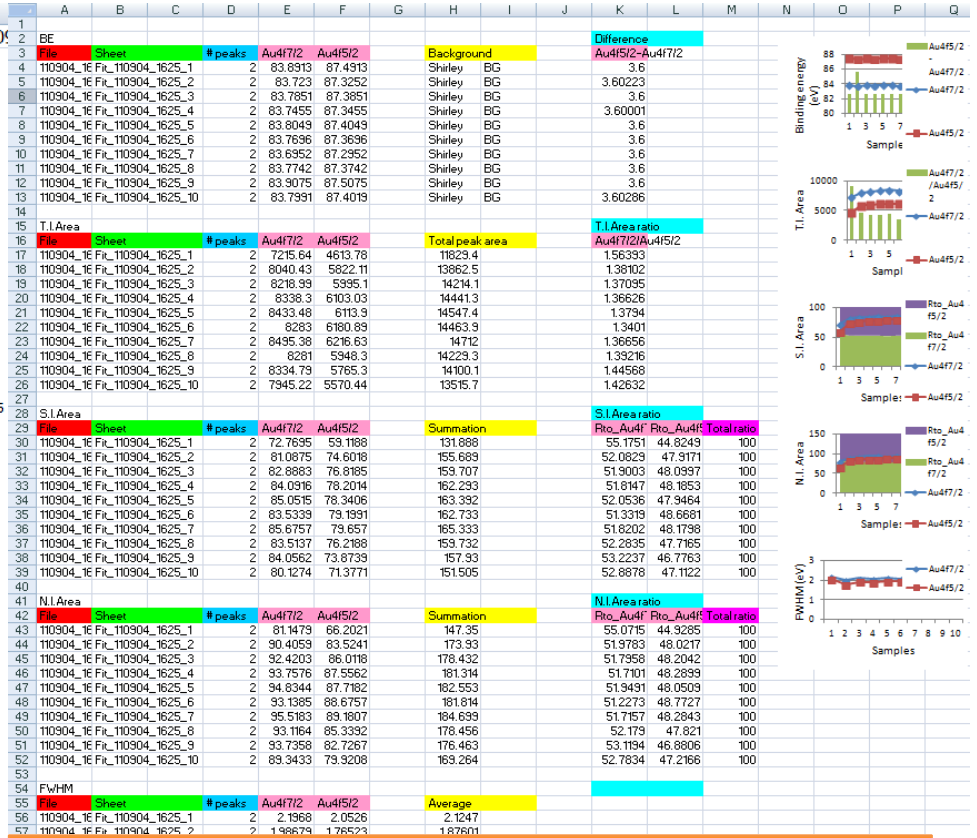
	A	B	C	D	E	F
1	Shirley	BG		ana	Au4f7/2	Au4f5/2
2	Tolerance	0.000001		BE	83.89131	87.49132
3	Initial A	0.001		KE	509.1087	505.5087
4	Final A	0.00344		FWHM1	2.196802	2.052602
5	Iteration	6		FWHM2		



Summary of fitting results



	A	B	C	D	E	F	G	H	I	J
1		110904_1625_1.xlsx			110904_1625_2.xlsx			110904_1625_3.xlsx		
2										
3										
4	Shift	0 eV		Shift						
5										
6										
7										
8										
9	Offset/mu	0		1	Offset/					
10	BE / eV	Shift	In-BG		BE / eV					
11	97	97	24.01026							
12	96.9	96.9	-31.9686		9					
13	96.8	96.8	6.137477		9					
14	96.7	96.7	-30.8481		9					
15	96.6	96.6	4.181989		9					
16	96.5	96.5	-8.75868		9					
17	96.4	96.4	17.24916		9					
18	96.3	96.3	2.27888		9					



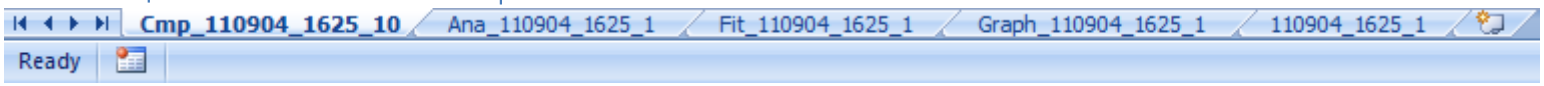
	A	B	C	D	E	F	G	H	I	J	K	L	M
1													
2	BE										Difference		
3	File	Sheet	# peaks	Au4f7/2	Au4f5/2		Background				Au4f5/2-Au4f7/2		
4	110904_1625_1	Fit_110904_1625_1	2	83.8913	87.4913		Shirley	BG			3.6		
5	110904_1625_2	Fit_110904_1625_2	2	83.723	87.3252		Shirley	BG			3.60223		
6	110904_1625_3	Fit_110904_1625_3	2	83.7851	87.3851		Shirley	BG			3.6		
7	110904_1625_4	Fit_110904_1625_4	2	83.7455	87.3455		Shirley	BG			3.60001		
8	110904_1625_5	Fit_110904_1625_5	2	83.8049	87.4049		Shirley	BG			3.6		
9	110904_1625_6	Fit_110904_1625_6	2	83.7696	87.3696		Shirley	BG			3.6		
10	110904_1625_7	Fit_110904_1625_7	2	83.6952	87.2952		Shirley	BG			3.6		
11	110904_1625_8	Fit_110904_1625_8	2	83.7742	87.3742		Shirley	BG			3.6		
12	110904_1625_9	Fit_110904_1625_9	2	83.9075	87.5075		Shirley	BG			3.6		
13	110904_1625_10	Fit_110904_1625_10	2	83.7991	87.4019		Shirley	BG			3.60286		
14													
15	T.I.Area										T.I.Area ratio		
16	File	Sheet	# peaks	Au4f7/2	Au4f5/2		Total peak area				Au4f7/2/Au4f5/2		
17	110904_1625_1	Fit_110904_1625_1	2	7215.64	4613.78		11829.4				1.56393		
18	110904_1625_2	Fit_110904_1625_2	2	8040.43	5822.11		13862.5				1.38102		
19	110904_1625_3	Fit_110904_1625_3	2	8218.99	5995.1		14214.1				1.37095		
20	110904_1625_4	Fit_110904_1625_4	2	8338.3	6103.03		14441.3				1.36626		
21	110904_1625_5	Fit_110904_1625_5	2	8433.48	6113.9		14547.4				1.3794		
22	110904_1625_6	Fit_110904_1625_6	2	8283	6180.89		14463.9				1.3401		
23	110904_1625_7	Fit_110904_1625_7	2	8495.38	6216.63		14712				1.36656		
24	110904_1625_8	Fit_110904_1625_8	2	8281	5948.3		14229.3				1.39216		
25	110904_1625_9	Fit_110904_1625_9	2	8334.79	5765.3		14100.1				1.44568		
26	110904_1625_10	Fit_110904_1625_10	2	7945.22	5570.44		13515.7				1.42632		
27													
28	S.I.Area										S.I.Area ratio		
29	File	Sheet	# peaks	Au4f7/2	Au4f5/2		Summation				Rto_Au4f	Rto_Au4f5	Total ratio
30	110904_1625_1	Fit_110904_1625_1	2	72.7695	59.1188		131.888				55.1751	44.8249	100
31	110904_1625_2	Fit_110904_1625_2	2	81.0875	74.6018		155.689				52.0829	47.9171	100
32	110904_1625_3	Fit_110904_1625_3	2	82.8883	76.8185		159.707				51.9003	48.0997	100
33	110904_1625_4	Fit_110904_1625_4	2	84.0916	78.2014		162.293				51.8147	48.1853	100
34	110904_1625_5	Fit_110904_1625_5	2	85.0515	78.3406		163.392				52.0536	47.9464	100
35	110904_1625_6	Fit_110904_1625_6	2	83.5339	79.1991		162.733				51.3319	48.6681	100
36	110904_1625_7	Fit_110904_1625_7	2	85.6757	79.657		165.333				51.8202	48.1798	100
37	110904_1625_8	Fit_110904_1625_8	2	83.5137	76.2188		159.732				52.2835	47.7165	100
38	110904_1625_9	Fit_110904_1625_9	2	84.0562	73.8739		157.93				53.2237	46.7763	100
39	110904_1625_10	Fit_110904_1625_10	2	80.1274	71.3771		151.505				52.8878	47.1122	100
40													
41	N.I.Area										N.I.Area ratio		
42	File	Sheet	# peaks	Au4f7/2	Au4f5/2		Summation				Rto_Au4f	Rto_Au4f5	Total ratio
43	110904_1625_1	Fit_110904_1625_1	2	81.1479	66.2021		147.35				55.0715	44.9285	100
44	110904_1625_2	Fit_110904_1625_2	2	90.4059	83.5241		173.93				51.9783	48.0217	100
45	110904_1625_3	Fit_110904_1625_3	2	92.4203	86.0118		178.432				51.7958	48.2042	100
46	110904_1625_4	Fit_110904_1625_4	2	93.7576	87.5562		181.314				51.7101	48.2899	100
47	110904_1625_5	Fit_110904_1625_5	2	94.8344	87.7182		182.553				51.9491	48.0509	100
48	110904_1625_6	Fit_110904_1625_6	2	93.1385	88.6757		181.814				51.2273	48.7727	100
49	110904_1625_7	Fit_110904_1625_7	2	95.5183	89.1807		184.699				51.7157	48.2843	100
50	110904_1625_8	Fit_110904_1625_8	2	93.1164	85.3392		178.456				52.179	47.821	100
51	110904_1625_9	Fit_110904_1625_9	2	93.7358	82.7267		176.463				53.1194	46.8806	100
52	110904_1625_10	Fit_110904_1625_10	2	89.3433	79.9208		169.264				52.7834	47.2166	100
53													
54	FWHM												
55	File	Sheet	# peaks	Au4f7/2	Au4f5/2		Average						
56	110904_1625_1	Fit_110904_1625_1	2	2.1968	2.0526		2.1247						
57	110904_1625_2	Fit_110904_1625_2	2	1.98679	1.76523		1.87601						

Cmp sheet: BG subtracted spectra

Ana sheet: BE, Peak areas, FWHM

Rto sheet can be generated from this sheet if all elemental peak fitting results prepared for atomic ratio analysis.

T.I. area: Trapezoidal integration of peak area
S.I. area: T.I. area normalized with RSF
N.I. area: T.I. area normalized with corr. RSF



Enjoy!

Depth-profile XPS: RSC Adv. 6, 94905 (2016).