EX3ms cheat sheet

Worksheet function and command reference (color code: pub, std, adv)

Hideki NAKAJIMA, rev. 12 Nov. 2021

Working conditions

OS: Windows MS Office 365 or later 2007/macOS MS Office 16
Max characters on filename without extension: 11
Directory and filenames restrictions: English
Decimal and thousand symbols: "." and "," respectively

Functions in the sheet

Sheet name	Description	Extracted data
Data	Original data	
Graph	Plots in binding and kinetic energies	From data sheet
Check	Plots in each scan	From data sheet by "No" command
Time	Plots in time scale and fluence analysis	From data sheet by "Obb" command
Fit	Background subtraction and peak Fitting	From graph sheet
Ana	A summary of fitting results	From fit sheets
Cmp	A summary of BG subtracted profiles	From fit sheets
Rto	A summary of areas from Ana report	From ana sheets
Photo	Plots of XAS data	From data sheet
Exp	Data table exported from graph sheet	From graph sheet
Eck	Data table exported from check sheet	From check sheet
Norm	Data normalized	From graph sheet
Diff	Data subtracted	From graph sheet
Edge	Pre and post-edge correction	From graph sheet
Lcmb	Linear combination fit	From graph sheet
Graph_Norm	Plots based on the Norm sheet	From norm sheet
Fit_Norm	Peak fitting based on the Norm sheet	From graph_norm sheet
Graph_Edge	Plots based on the Edge sheet	From edge sheet
Fit_Edge	Peak fitting based on the Edge sheet	From graph_edge sheet
Graph_Lcmb	Plots based on the Lcmb sheet	From lcmb sheet
Fit_Lcmb	Peak fitting based on the Lcmb sheet	From graph_lcmb sheet
Pyt	Lmfit python script for curve fit	From Fit sheet
Calc	Simulation parameters	
Sim	Simulated data	From Calc sheet

Vms	Data table exported in VAMAS format	From Graph sheet by "vms" or "vamas"
VAMAS	Data imported from VAMAS format	
PEG	Data loaded from PEG simulation	(grating efficiency simulation)
Exp_Fit	Data exported from Fit sheet	From Fit sheet by "exp" command Run macro to export txt by Monte Carlo methods
Err	Standard error analysis of fitting	From Fit sheet by "error" command

Manual data load format template

Technique	Trigger in A1	Queries	Graph x-axis	Fitting
PES	KE/eV	PE & elements	BE & KE	Yes in BE scale
XPS	BE/eV	PE & elements	BE & KE	Yes in BE scale
XAS	PE/eV	Elements	PE	Yes in PE scale
Grating scan	GE/eV	Gap/1st har.& e	PE	No
AES	AE/eV	Elements	EE & dN/dE	No
RGA	QE/eV	*NA*	Mass	Yes in mass
Manual scan	ME/eV	*NA*	Position	Yes in x
Histogram	HE/eV	*NA*	Position	Yes in x
Photodiode	FE/eV	Gap/1st har.	PE	No

Command list in each sheet

Command	Cell	Sheet	Result
chem	C10	Graph, Cmp	Chemical shifts
elem	C10	Graph	Revise elements
intp	A1	Data	Interpolate data by B1 value
ana	C10	Graph	Update Fit sheet
exp	A1	Graph, Check, Cmp	Export data with "E/eV" labels for X axis (used to export each data into text file)
expo	A1	Graph, Check, Cmp	Export data with filename-related X axis (used to paste it in Origin program or the others)
expk	A1	Graph	Export data with "KE/eV" kinetic energy axis
comp	D1	Graph	Compare the spectra
auto	A1	Graph, Cmp	Calibrate offset and multiple factors (see the detailed functions below)
cali(*p*)	A1	Graph	Fit C1s peak position at 284.6 eV (*p*: poly bg)
noise(*n*)	A1	Graph	Remove shot noise when S/N > *n* (default 5)
peg	A1	Graph	Compare har+1 on PEG simulation file
ana	D4	Fit	Summarize Fit sheets
ana	A1	Ana	Summarize Ana sheets into Rto sheet
exp	A1	Check	Export data to be imported into elsewhere

exp	A1	Cmp	Export data to be imported into elsewhere
char	A1	Graph	Apply char for each workbook
	A1 & C1, … = "KE/eV"	Eck	Export text data files for each two-column
debug	A1	Graph	Apply the same graph parameters to files
debug	D1	Fit	Apply the same fit parameters from text files
debugn	A1	Graph	Add reference data to be normalized
debuga	D1	Fit	Apply previous fit parameters from text files
debugf	D1	Fit	Apply RSF in the fit sheet only
debugc	D1	Fit	Apply fit parameters in the fit sheet only
debugp	D1	Fit	Apply previous fit parameters on fit sheet
exp	D1	Fit	Export fit data in to Exp sheet
expbn	D1	Fit	Add b to export BG, add n to rename data
error	D1	Fit	Evaluate standard error by chi^2 +/-1
monte	D1	Fit	Evaluate area SD by Monte Carlo method
strap	D1	Fit	Evaluate area SD by Bootstrap method
mean*X*	C1	Exp_Fit	Export *X* csv files by Monte Carlo/Bootstrap
norm, diff	A1	Graph	Normalize first data by second added data
cked	A1	Graph	Normalized by gold C K edge in database
edge	A1	Graph	Pre and post edge correction.
lcmb	A1	Graph	Linear combination of multiple spectra
		Time	Fluence analysis interpolated in any points
vms	A1	Graph	Single export in vamas format
vamas	A1	Graph	Multiple regions export in vamas format
phi	A2	Data	Export and plot from Multipak exported csv
multi	A2	Data	Plot graph from Multipak exported csv
simulation	A1		Simulate the spectrum with elements
lmfit	A4	Fit	Export Python code for lmfit

Backgrounds in the fit sheet

Type of BG	A1	B1	C1
Shirley BG	sh	ab/bg	
Tougaard BG	to	bg	
Polynomial BG	po	ab/bg	
Polynomial Normal BG	po	no	ab/bg
Polynomial Shirley BG	po	sh	ab/bg
Polynomial Tougaard BG	po	to	ab/bg
Polynomial Edge BG	po	ed	ab/bg
Polynomial AsLS BG	po	as	ab/bg
Slope Shirley BG	sl	sh	ab/bg
Shirley Iterated BG	sh	it	bg
Shirley Peak BG	sh	pe	abg
Shirley Virtual BG	sh	vi	ab/bg
Arctan BG	ar	ab/bg	
Erf BG	er	ab/bg	

Victoreen BG	vi	ab/bg	
Double Exponential BG	do	ab/bg	
Lognormal	lo	ab/bg	
Sigmoid fit + spline BG	si	fi	
Sigmoid convoluted fit	si	co	fi
Double Sigmoid fit	do	si	fit
User-defined function	ud	fit	
SAXS	sa	fit	
CK (based on Arctan BG)	ck		

Peak shapes in the fit sheet

Syntax	Shape	Option a	Option b	#par	Ref.
G (0)	Gaussian			3	
DB G (0)	Double Gaussian			4	Fityk
EMG	Exponentially Modified Gaussian	Distortion para.		4	Fityk
L (1)	Lorentzian			3	
DS L (1)	Doniac-Sunjic x L	Asymmetric para.		5	CasaXPS
DB L (1)	Double Lorentzian			4	AAnalyzer
PEA	Pearson VII	Skewness		4	Fityk
SGL, PGL (0-1)	G + L, G x L (pseudo-Voigt)			5	Unifit CasaXPS
ASGL, APGL	Asymmetric V Double Voigt			5	10.1107/ S0021889884011043
ESGL, EPGL	Exponential blended Voigt	Exponential decay parameters		5	CasaXPS
DS SGL, DS PGL	DS x L blended V	Asymmetric parameter	Ratio DSL:V	6	CasaXPS
UG SGL, UG PGL	Ulrik Gelius blended Voigt	Asymmetric parameter a	Asymmetric parameter b	6	CasaXPS
DSV SGL, DSV PGL	DS x Voigt blended Voigt	Asymmetric parameter	Ratio DSV:V	6	CasaXPS
TSGL	Exponential blend SGL (MultiPak)	Tail scale	Tail length at half max	6	MultiPak
GL (0 <	G + L with the			4	MultiPak

shape < 1)	same FWHM (MultiPak)				Eq. to SGL
MSGL	Asymmetric V	Asymmetric parameter	Sigmoid-center translation	6	10.1002/sia.5521
CGL	Numerical convolution G x L			4	10.1002/sia.2527
F	Fano profile			4	10.1103/PhysRev.124.1866
FG	F x G			5	
LOGN	Log normal	Mean (μ)		4	

Optimization mode of fittings

Cell in Fit sheet	Syntax or Font style	Optimization
BE, FWHM, Ampl, Shape, Options	Figures with Bold	Constraints
A14	Solve chi^2*	Least chi square
A14	Solve Abbe	Abbe criteria
A10 (EF fit)	Solve FD without Italic	Least chi square
A10 (EF fit)	Solve FD with Italic	Abbe criteria
A11 (EF fit)	Solve GC without bold	Gaussian convolution after FD + polynomial BG
A11 (EF fit)	Solve GC with bold	FD + Polynomial BG first, Gaussian convolution together with FD + poly BG

Calibrations in offset/multiple factors

A1 cell syntax in Graph sheet	Offset factor	Multiple factor
auto0	Set to 0	Set to 1
auto or auto1	First point to be zero	End point to be unity
auto10	Zero at point 10 from start point	Unity at point 10 from end point
auto(1,10)	Zero from point 1 to 10 from start point	Unity from point 1 to 10 from end point
auto[100:101,200:201]	Zero in BE range between 100 and 101 eV	Unity in BE range between 200 and 201 eV
automax / autowf	Zero at the lower side of a point of data	Unity at max intensity point of data
autop	Syntax previously done	Syntax previously done
auto{284.6}	BE at max. intensity to be calibrated in 284.6 eV	NA (BE calibration by Charging factor)
auto'-7.8'	Charging correction at -7.8 eV	NA (this is based on C1s BE

	for all spectra	calibration)
offset10	Offset spectra for water fall plot	NA

List of element groups to be identified

Code	Group	Elements to be analyzed
AL	Alkali metals	Na,K,Rb,Cs
EA	Alkaline Earth metals	Be,Mg,Ca,Sr,Ba,Ra
TM	Transition metals	*3d + 4d + 5d transition metals*
3d	3d transition metals	Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu,Zn
4d	4d transition metals	Y,Zr,Nb,Mo,Tc,Ru,Rh,Pd,Ag,Cd
5f	5d transition metals	Lu,Hf,Ta,W,Re,Os,Ir,Pt,Au,Hg
SM	Semi-metals	B,Si,Ge,As,Sb,Te
NM	Non-metals	C,N,O,P,S,Se
BM	Basic metals	Al,Ga,In,Sn,Tl,Pb,Bi
HA	Halogens	F,Cl,Br,I,At
NG	Noble gases	Ne,Ar,Kr,Xe,Rn
RM	Rare metals	La,Ce,Nd,Sm,Eu,Gd,Tb,Er,Tm,Yb,Th,U
LA	Lanthanides	La,Ce,Nd,Sm,Eu,Gd,Tb,Er,Tm,Yb
AC	Actinides	Th,U

Advanced syntax templates in the sheets

	Sheet	Cells	Formula	Reference	Calibrated #1	Calibrated #2
Extra photons	Graph	C2	;100;200;333 eV			
Specific scans	Graph	B8	[1,2-4]			
Amp ratio	Fit	D14-	(4;3)	(4;	1;	3)
BE diff	Fit	D15-	[3.5;n3.5]	[	3.5;	n3.5]

Note1: "n" represents negative shift from reference.

Note2: Empty cells between brackets does not affect to the constraints.

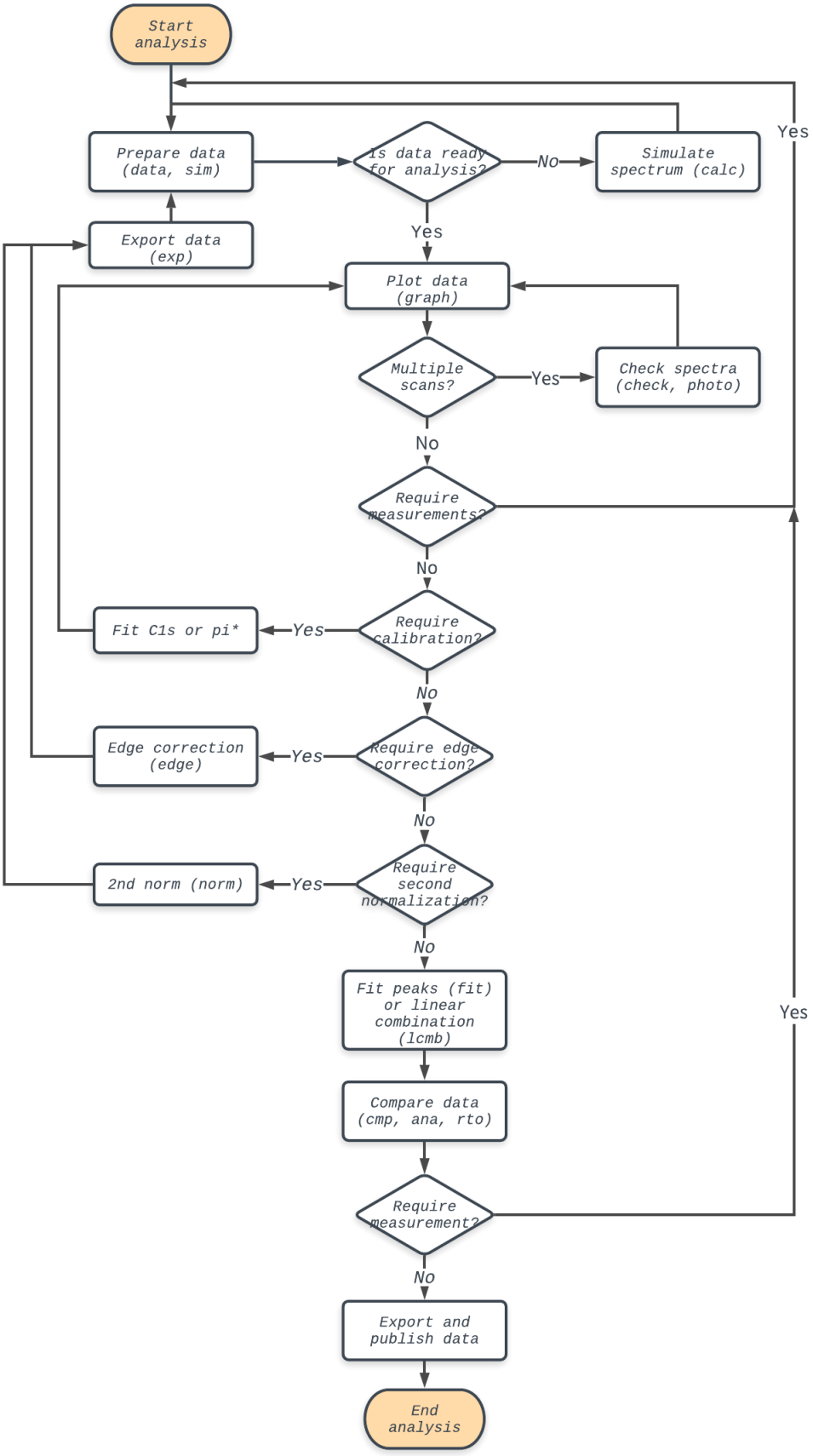
List of Peak area

	Usages	Descriptions	Factors to be effective
P. Area	Chemical state analysis	Peak area calculated with analytical formula and without any factors	Amplitude, FWHM
S. Area	Quantification of elements under the same condition	Peak area normalized with atomic sensitivity factor based on photo-ionization cross-section	Amplitude, FWHM, PE, Sensitivity based on element specified in the *Graph* sheet

N. Area	Quantification of elements under the various measurement conditions	Peak area calculated in "S. Area" plus normalized with empirically calculated factors at BL CLAM2 including XPS mean-free path of photoelectrons, transmission function of electron energy analyzer based on pass energy, grating efficiency	Amplitude, FWHM, PE, KE, Sensitivity, CAE, Grating, MFP factor, a & b specified in the *Fit* sheet based on formalism from CasaXPS Corr. RSF is used to evaluate the area from P

T.I./S.I./N.I. are numerically integrated areas with Trapezoidal rule applied to each corresponding area shown above.

Workflow


Start analysis
Prepare data (data, sim)
Is data ready for analysis?
No
Simulate spectrum (calc)
Yes
Export data (exp)
Yes
Plot data (graph)
Multiple scans?
Yes
Check spectra (check, photo)
No
Require measurements?
Yes
No
Fit C1s or pi*
Yes
Require calibration?
No
Edge correction (edge)
Yes
Require edge correction?
No
2nd norm (norm)
Yes
Require second normalization?
No
Fit peaks (fit) or linear combination (lcmb)
Compare data (cmp, ana, rto)
Require measurement?
Yes
No
Export and publish data
End analysis