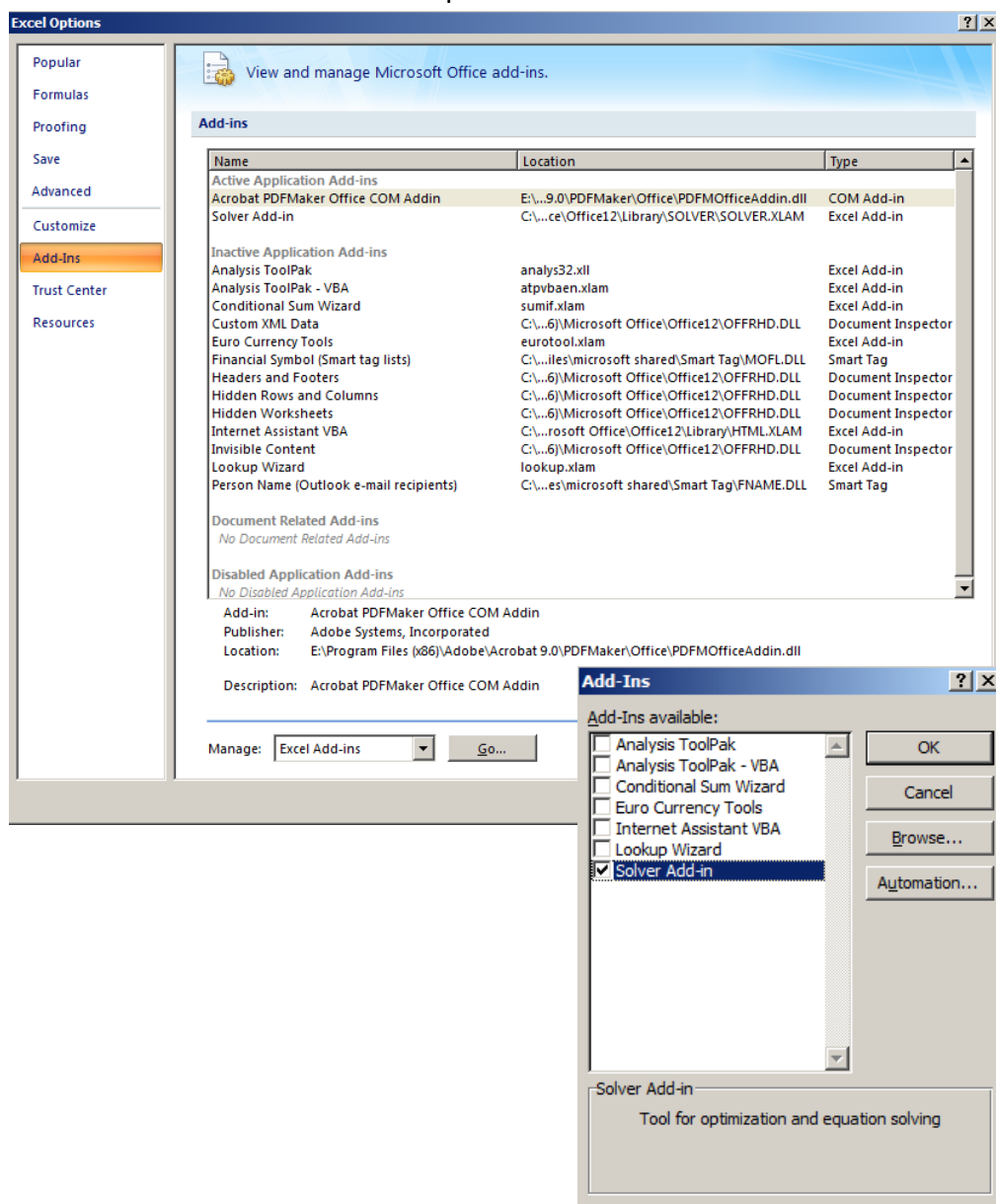
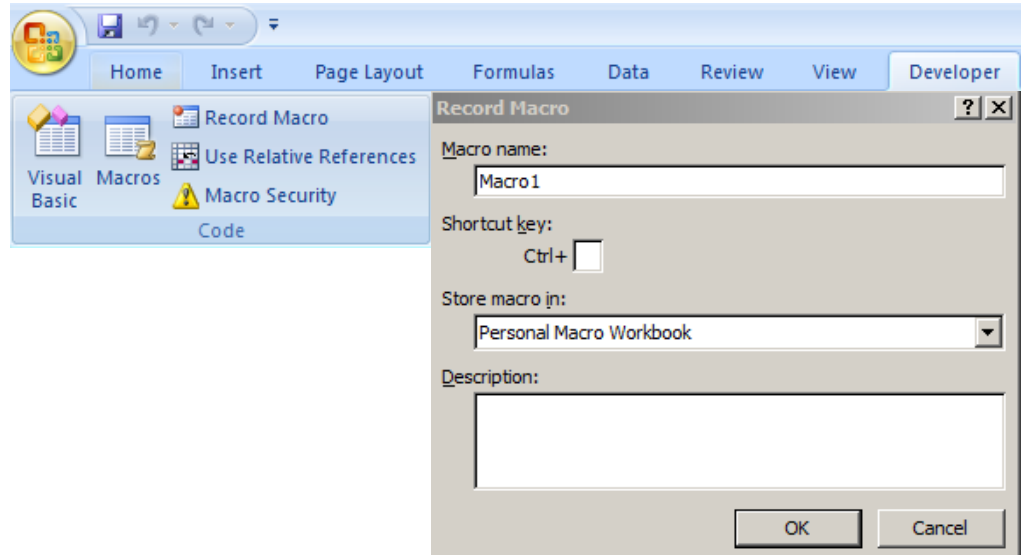


Peak-fitting procedures on XPS data by Excel

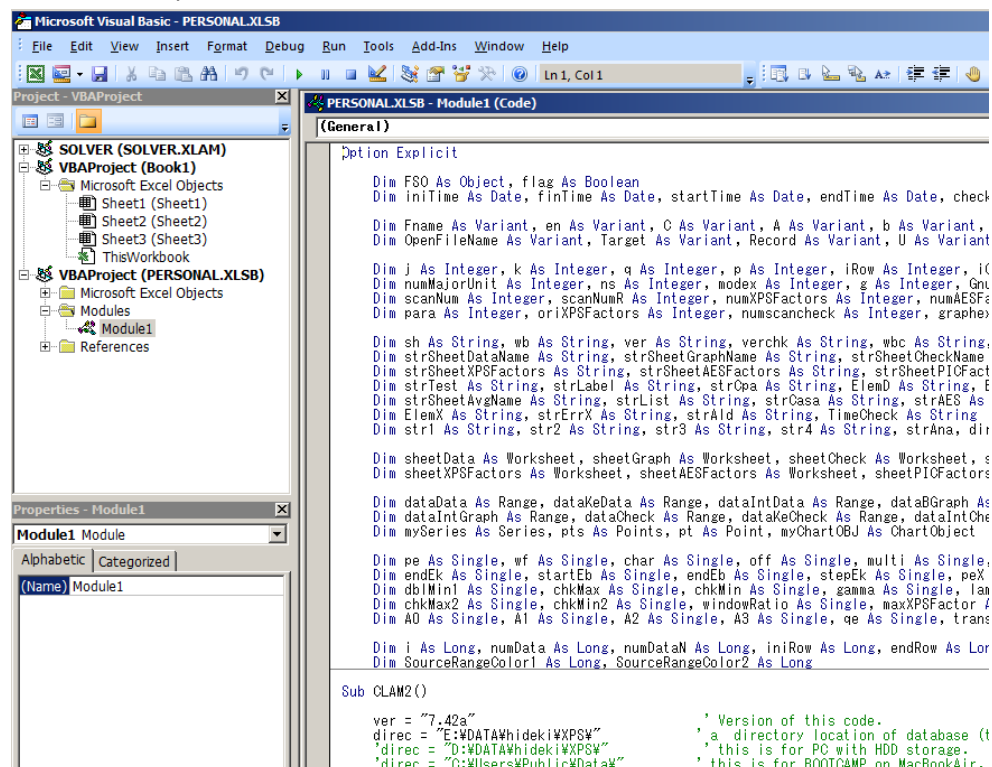
1. Get the Excel XPS macro code on GitHub.
<https://github.com/heitler/xps-excel-macro>
2. Install the Visual Basic for Applications (VBA) code developed by Hideki and Solver add-ins in Excel.
 - a. Install **Solver add-ins** from Excel Options - Add-Ins - Go... - Solver Add-in.



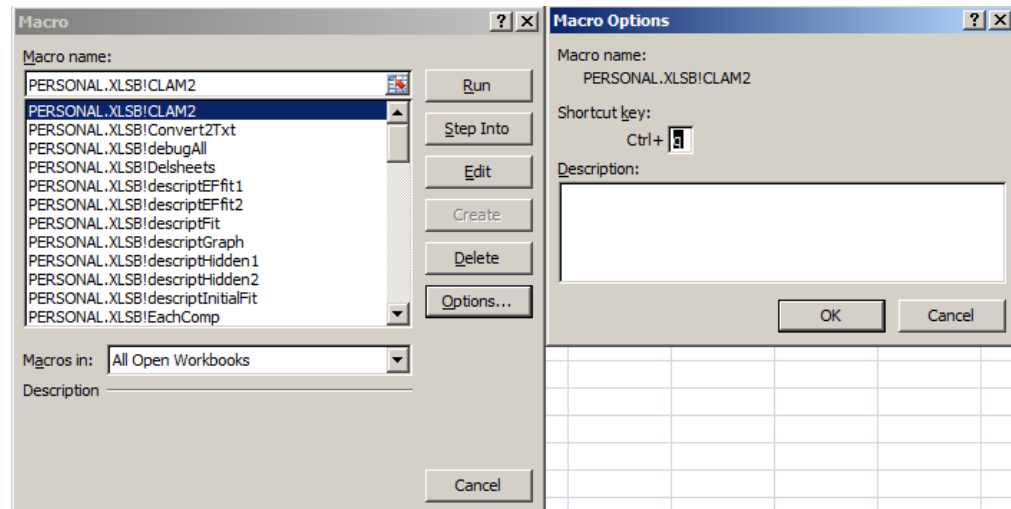
- b. Create a Personal Macro Workbook (**personal.xlsb**).
 - i. Show Developer tab in the Ribbon in Excel Options - Popular
 - ii. Record Macro from Developer tab by any name.
 - iii. Store macro in: "Personal Macro Workbook"
 - iv. Stop Recording from Developer tab



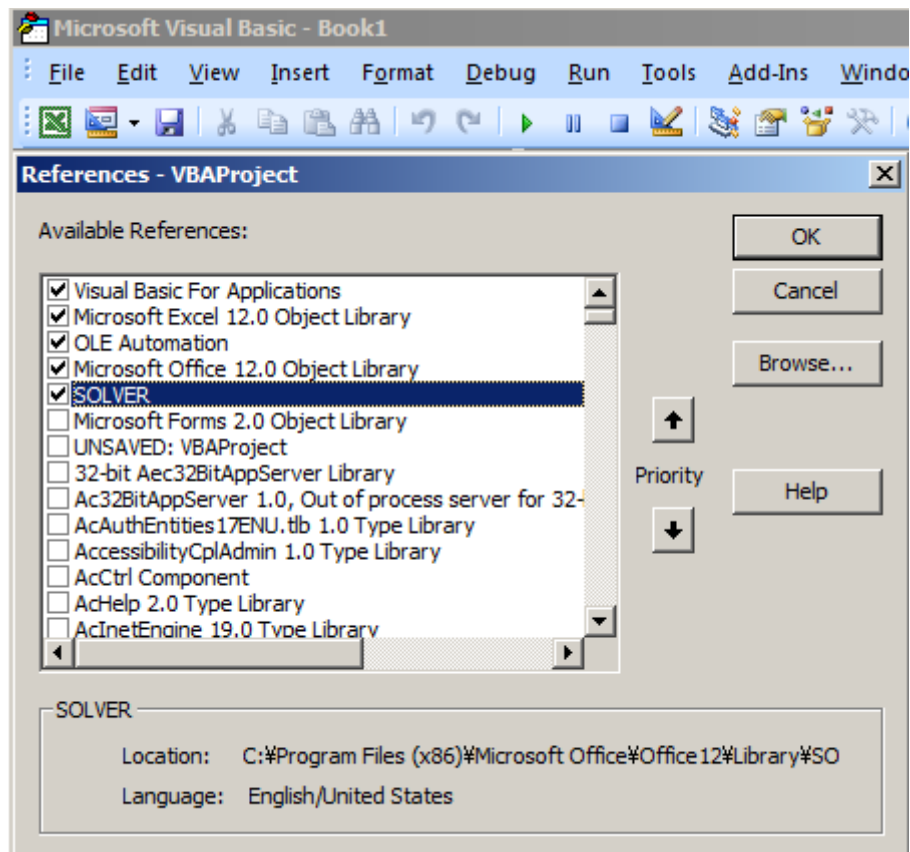
- c. Copy and paste the VBA code (personal.xlsb) into your personal.xlsb (VBAProject - Modules - Module1) from VBA editor (Alt+F11 or Developer tab - Visual Basic).



- d. Assign the shortcut keys (**Ctrl + q**) for the VBA code from Developer tab - Macros - Personal.xlsb!CLAM2 - Options... - Shortcut key: Ctrl + "q".



- e. Check Solver add-ins library in the VBAProject references from VBA editor - Tools - Solver.



- f. Copy and paste your own database (if you have any) into the folder specified in the VBA code (default folder: D:\Data\hideki\XPS\). WebCross folder is also in the same place (default folder: D:\Data\hideki\XPS\webCross\). If you have no database files or folders, the user-defined database workbook will be generated automatically in the first run of the VBA code as a filename "UD.xlsx", and then you can modify or add your elements with binding energy and sensitivity factors for AlKa. The binding energy data is necessary, for example, from the link below.

<https://userweb.jlab.org/~gwyn/>

No sensitivity factor is necessary if webcross folder includes data specified below. Cross-section database files in webCross folder is also necessary to normalize the photon energy dependent cross section if the XPS photon energy is not AlKa.

<https://vuo.elettra.eu/services/elements/data/>

3. Import data in Excel.

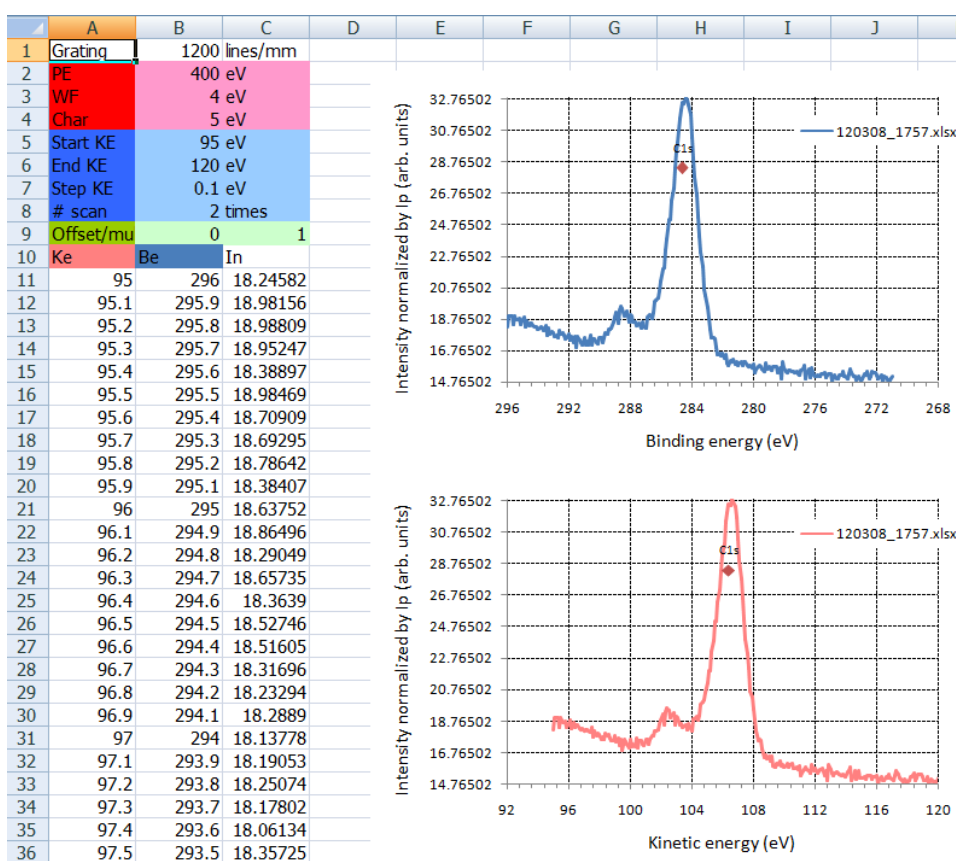
- a. Save tab-delimited texts or spreadsheet file with KE/BE scale in the first column and spectral intensity in the second column. The first line of the first column should be either "KE/eV" for kinetic energy or "BE/eV" for binding energy in XPS. XAS used to be "PE/eV". The first line of the second column should be either "AlKa" for 1486.6 eV of photon energy or empty for dialog to be asked for photon energy used.

	A	B	C
1	BE/eV	AlKa	
2	382	19655	
3	381.9	19555	
4	381.8	19215	
5	381.7	20310	
6	381.6	19330	
7	381.5	18845	

- b. Open the text data file or workbook with Excel (right-click on text file).
- c. Run the VBA code by the shortcut key (Ctrl + q).
 - i. Note that run the VBA code to update the analysis, plot or fitting after you revise any parameters in the following process.
 - ii. Each sheet has a number of useful commands to be analyzed in details, but it can be learned afterwards.

- d. Input the atomic elements to be analyzed and shown up in graphs.

4. Calibrate the binding energy (BE) of spectrum by changing photon energy (PE), work function (WF), and charging factor (Char).
- Compare the standard data (XPS standard BE database given by **red marker**) or spectrum (C1s peak as *adventitious* carbon) to calibrate the binding energy.
 - Change numbers to shift the spectrum in B2:B4 cells as specified.
 - Spectra can be compared by typing "*comp*" with Ctrl + q (Select the Excel files to be compared after the shortcut key).
 - Change Offset or Multiple factors in B9:C9 cells to scale the spectral intensity.
 - Show the standard chemical shifts by "*chem*" in C10 cell with Ctrl + q.



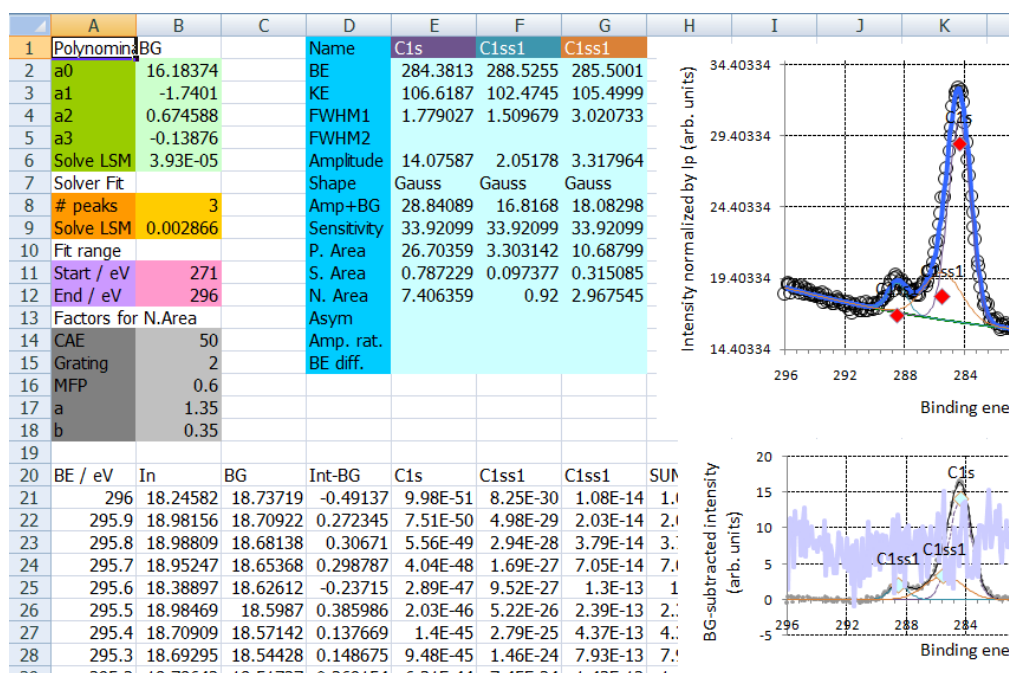
5. Fit peaks based on the element identified with binding energy calibrated in the Graph sheet.
- Set up the background shape by typing following in A1 and A2 cells.
 - A1 for "s" to Shirley's BG (default)
 - A1 for "t" to Tougaard's BG

- iii. A1 for "p" to Spline BG (including constant and linear)
 - iv. A1 for "s" and A2 for "s" to Spline Shirley BG
 - v. A1 for "s" and A2 for "t" to Spline Tougaard BG
 - vi. A1 for "v" to Victoreen BG used for XAS
 - vii. A1 for "a" to Tangent Arc BG used for XAS
 - viii. A1 for "e" to fit the Fermi edge.
- b. Set up the fitting binding energy range in B11 and B12 cells.
- c. Set up peak amplitude (E6,F6,...), FWHM (E4,...), BE (E2,...), and number of peaks (B8). Note that the parameters can be fixed as constraints with bold type face on each number.
- d. Setup peak shape in E7, F7, ... cells as follows;
- i. "0" or "Gauss" for a normal distribution
 - ii. "1" or "Lorentz" for a Cauchy distribution
 - iii. Any value between 0 and 1 or "Voigt" for pseudo-Voigt function (*italic type face on numbers for asymmetric function*)
 - iv. More peak shapes available from Form cells like G, L, GL, TSGL.
- e. Setup amplitude ratios and BE differences if desired.

Name	C1	C2	C3
Amp. rat.	(2;	1)	
BE diff.	[0.1;	0.2]

Table description above means that amplitude ratio between C1 and C2 peaks is 2:1 and the binding energy differences among C1, C2, and C3 are 0.1 and 0.2 eV, respectively.

- f. The differences in three peak areas are summarized in the table below. The corresponding three numerical Trapezoidal integration areas are also shown.



	Usages	Descriptions	Factors to be effective
P/T.I. Area	Single-element peak	Peak area calculated without any factors	Amplitude, FWHM
S. Area	Multiple-element peaks	Peak area calculated with atomic sensitivity factor based on photo-ionization cross-section	Amplitude, FWHM, PE, Sensitivity based on element specified in graph sheet
N. Area	Multiple-element peaks measured under different BL or analyzer 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 based on formalism from CasaXPS

6. Sample analysis after the fitting on each spectrum.

- Compare the peak areas and shifts based on the fitting results by typing "*ana*" in D1 cell with Ctrl + q at Fit sheet (Select Excel files to be compared).

