This is a brief instruction for using the DLS I09 Scilab script to analyse XSW data (by Tien-Lin Lee on 18/03/2015).

To use the Scilab script to analyse XSW data you need to

(a) download and install the latest stable version of Scilab

(b) place the following file in a folder (specified by 'script_dir' in the script):

(1) nff file(s) for the substrate (one for each element); can be downloaded at http://henke.lbl.gov/optical_constants/sf/sf.tar.gz

(2) 'si.nff' (for the Si monochromator).

(3) 'f0_all_free_atoms.txt'; contact DLS I09 if you need a copy.

(4) 'trzhaskovskaya_at_data_nucl_data_tab.txt' (for non-dipolar corrections); contact DLS I09 if you need a copy.

(c) Define the crystal structure of the sample substrate:

```
95    lps0=[4.08516,4.08516,4.08516,90,90,90];
                        // a, b and c in angstrom; alpha, beta and gamma in deg, sample.
96    DWBs=0; // Debye-Waller B factor, sample.
97    xyzs=[
98    47,0,0,0,1; // Atomic number, atomic coordinate x, y, z, occupancy
99    47,0.5,0.5,0,1;
100   47,0.5,0,0.5,1;
101   47,0,0.5,0.5,1;];
```

(d) ensure the presence of the data files required by the XSW script:

(1) Reflectivity data file – a two-column text file (1st column: photon energy in eV; 2nd column: reflectivity). The photon energy steps do not need to be evenly spaced.

(2) XPS data file – a multi-column text file. A photon energy column is not needed but the energy steps must match exactly those in the reflectivity data file.

At DLS I09, a reflectivity data file is prepared by another Scilab script 'nxs3D2txt'. The reflectivity file should have a name like 'i09-XXXXX-r.txt', if it is extracted from a single scan, or 'i09-XXXXX-XXXXX-r.txt', if it is extracted from several scans. XPS data files are usually output from CasaXPS. All these data files should be stored in a folder '.../i09-XXXXX-txt/' or '.../i09-XXXXX-XXXXX-txt/' created by 'nxs3D2txt'. The data file name and folder to be defined in the present XSW script assume 'nxs3D2txt' is used. If this is not the case, the scripts following the variables 'dataprefix' (Line 11), 'datadir' (Line 12) and 'rfile' (Lin 72) in the XSW script may need to be modified.

(e) define the following variables for the data to be analysed:

```
10    script_dir="C:\TLLEE_1\Scilab-user-scripts\xsw script new\"; // Folder containing
11    dataprefix="i09-46053-46080"; // File prefix for reflectivity data (usually named by script
      'nxs3D2txt'); Extension should be '.txt';
12    datadir="C:\TLLEE_1\Manuscript\I09 HP Steinrueck\"+dataprefix+"-txt\"; // Folder containing
      reflectivity and xps data created by script 'nxs3D2txt'; replace this with the full path if the
      folder is named differently;
13    xpsfile="Co2p.TXT"; // Multi-column XPS data file; can be created by CasaXPS;
14    xpscol=7; // Column number in the XPS data file that contains the core-level data to be
      analysed
```

15 xpselem='Co'; // String, element to be analysed; case sensitive
16 xpscorelevel='2p3/2'; // String, core-level of the element to be analysed; case sensitive and no space
17 xpslabel="779.5eV_test"; // Additional label, e.g., binding energy, to be used to identify a chemical component
19 samp="Ag"; // Chemical formula of sample crystal; this does not affect the XSW calculations
20 hs=[0,0,2]; // Sample reflection
21 energy=3040; // Photon energy in eV
22 fwhmgaus=0.295; // in eV, FWHM of the Gaussian to be convoluted with the sample theoretical rocking curve (to account1 for, e.g., mosaicity).
23 fh0=0.6; // Initial value of coherent fraction
24 ph0=0.5; // Initial value of coherent position
25 NDC=1; // Non-dipolar corrections; On: NDC = 1; Off: NDC = 0.
27 hm=[1,1,1]; // Reflection of Si monochromator
28 N_monobounce=2; // Number of bounces of Si monochromator reflection; 2 for DCM and 4 for 4-bounce mono
36 thdeg=15 // Theta angle defined in FIG1 in Trzhaskovskaya (2001) (see below)

Note that

(1) 'script_dir' and 'datadir' must end with a '\';
(2) 'xpselem' is case sensitive; 'xpscorelevel' can be 1s, 2s, 2p1/2, 2p3/2, 3s, 3p1/2, 3p3/2, 3d3/2, 3d5/2 …;
(3) for most analysis Lines 27 and 28 do not need to be changed;
(4) the non-dipolar corrections use the parameters tabulated in Trzhaskovskaya et al., Atomic Data and Nuclear Data Tables **77**, 97 (2001), and **82**, 257 (2002). At I09 the electron analyser is oriented along the polarisation direction of the incident beam and capable of accepting ±30° in a horizontal plane. 'thdeg' in Line 36 is the emission angle of photoelectrons in the horizontal plane with respect to the polarisation direction. For the electrons collected over an angular range, 'thdeg' may be approximated by the centre of the range. For example, when a sample is facing the incident beam, only 'thdeg' between 0 and +30° is detectable (because the other half is blocked by the sample itself) and therefore one may set 'thdeg' = 15 for angle-integrated data.

(f) Press F5 to save and execute the script, which generates three output files:

(1) a pdf file with a figure of the data and the fits and a summary of the fits,
(2) a 4-column text file ('..._dat.txt') containing the data,
(3) a 4-column text file ('..._fit.txt') containing the best fits calculated in a finer step.

The 2nd, 3rd and 4th columns in the two text files, which correspond to the relative photon energy E-Ebragg (ev), reflectivity and photoelectron yield, respectively, can be used to produce a high quality figure for publication.

(g) Adjusting the initial values fh0 and ph0 may be necessary to obtain a good fit to the photoelectron yield data.

(h) Adjust the Gaussian width 'fwhmgaus' and repeat the above steps until the 'Energy range' reported by the analysis agrees with the experimental photon energy range of the XSW scan.