Quantification of SPECSLAB I Spectra

The quantification of XPS spectra obtained from SPECSLAB I includes a spectrometer response correction. To obtain the same quantification results from CasaXPS as are computed from SPECSLAB I the spectra must include the spectrometer response function, which in general is not the case. It is therefore necessary to include the SPECSLAB I spectrometer response function in the new VAMAS file at the time the SPECSLAB I files are converted through CasaXPS into the VAMAS format. The following describes the procedure for performing this task.

The objective is to create a configuration file containing a transmission correction curve for a given pass energy (PE). Each time a .exp file containing spectra is converted through CasaXPS, the configuration file is read and the appropriate curve is added to the spectra in the new .vms file. Once the transmission correct is added to the raw SPECSLAB I data, near identical quantification between the two systems is reproduced.

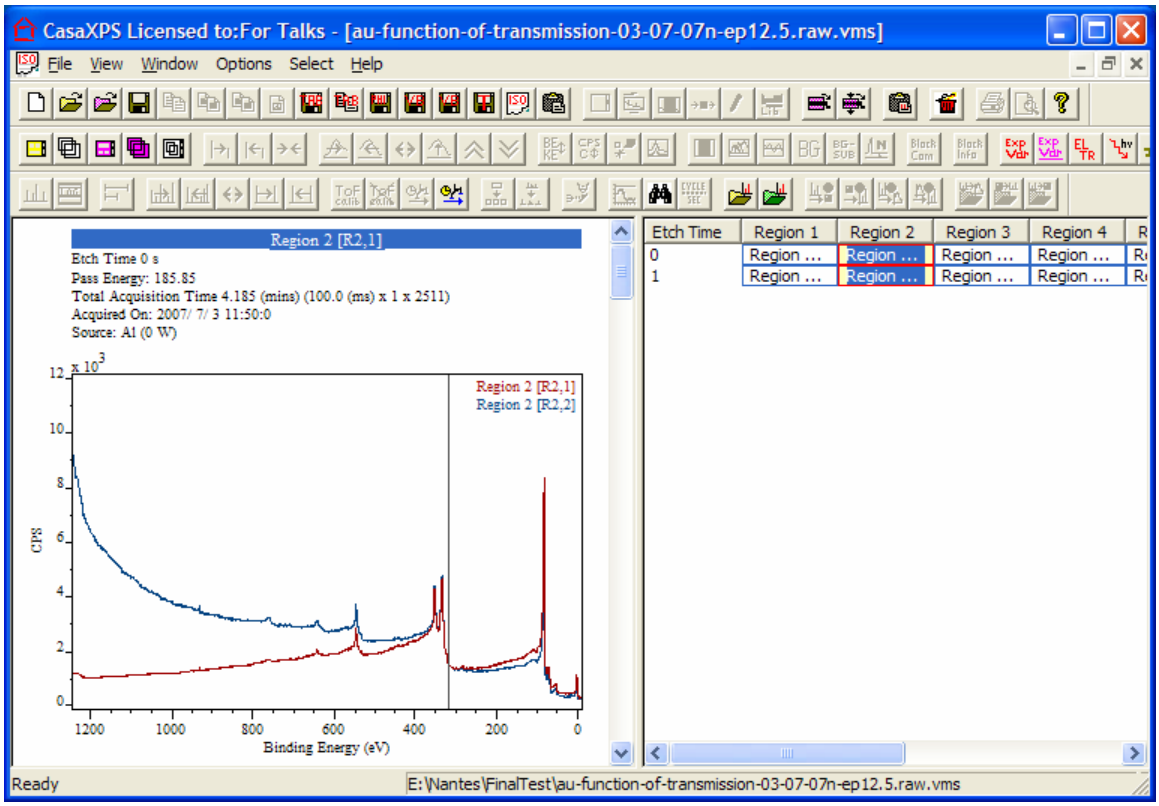


Figure 1: Survey spectra used to generate the transmission curve for PE126

Creating the Transmission Configuration File

To create the transmission correction file:

1. A .exp file must be prepared in SPECSLAB I where a set of survey spectra taken over as large a range of kinetic energies as possible using a range of pass energies, eg: PE 200.025, 185.85, 126, 89.775, 66.15, 50.4, 37.8, 31.7, 25.2 are prepared within a .exp file. The range of kinetic energies and pass energies should be chosen to ensure overlapping intervals in the value KE/PE for the set of spectra. The survey spectra must be processed in SPECSLAB I such that the spectra held in the .exp file are normalised using the spectrometer response-function. Once the data are processed, the .exp file will contain both the raw data and also the processed data.
2. Change the file extension of the .exp file containing the survey spectra to .raw and use CasaXPS version 2.3.14 to convert the SPECSLAB I data into VAMAS format. The newly created VAMAS file will contain two VAMAS blocks for each spectrum originally in the .exp file (Figure 1). The first of the two rows of VAMAS blocks will contain the processed spectra, while the second row contains VAMAS blocks of the corresponding raw data.
3. Assuming the VAMAS file contains two rows of corresponding VAMAS blocks containing valid processed and raw spectra, press the **Create SPECSLAB I TRF** button on the Test Data property page of the Spectrum Processing dialog window (Figure 2). A new Experiment Frame appears in which the transmission function curve for PE 126 is present.

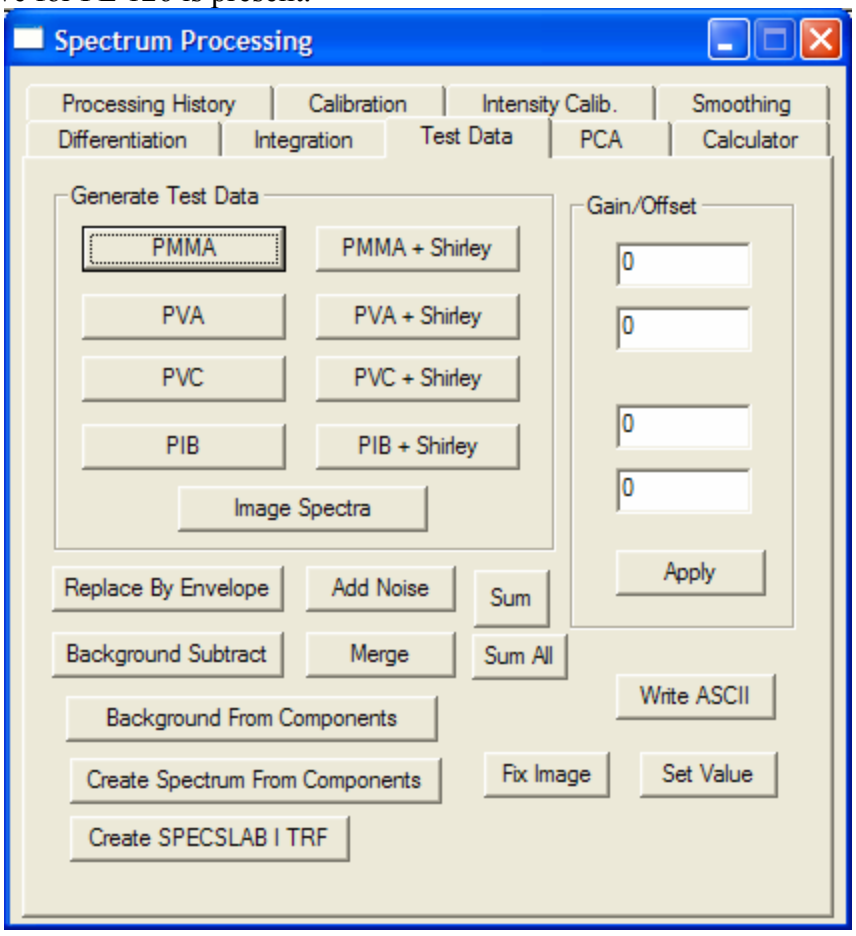


Figure 2: Test Data property page containing the Create SPECSLAB I TRF button.

4. After inspection of the resulting transmission curve (Figure 3), the Experiment Frame containing the newly created transmission function must be saved to the same directory as the CasaXPS.exe file with the name CasaXPS_SPECSLAB_I.trf. Each time a .exp file is converted, the curve within the CasaXPS_SPECSLAB_I.trf is used to add the appropriate correction to the data in the VAMAS file.

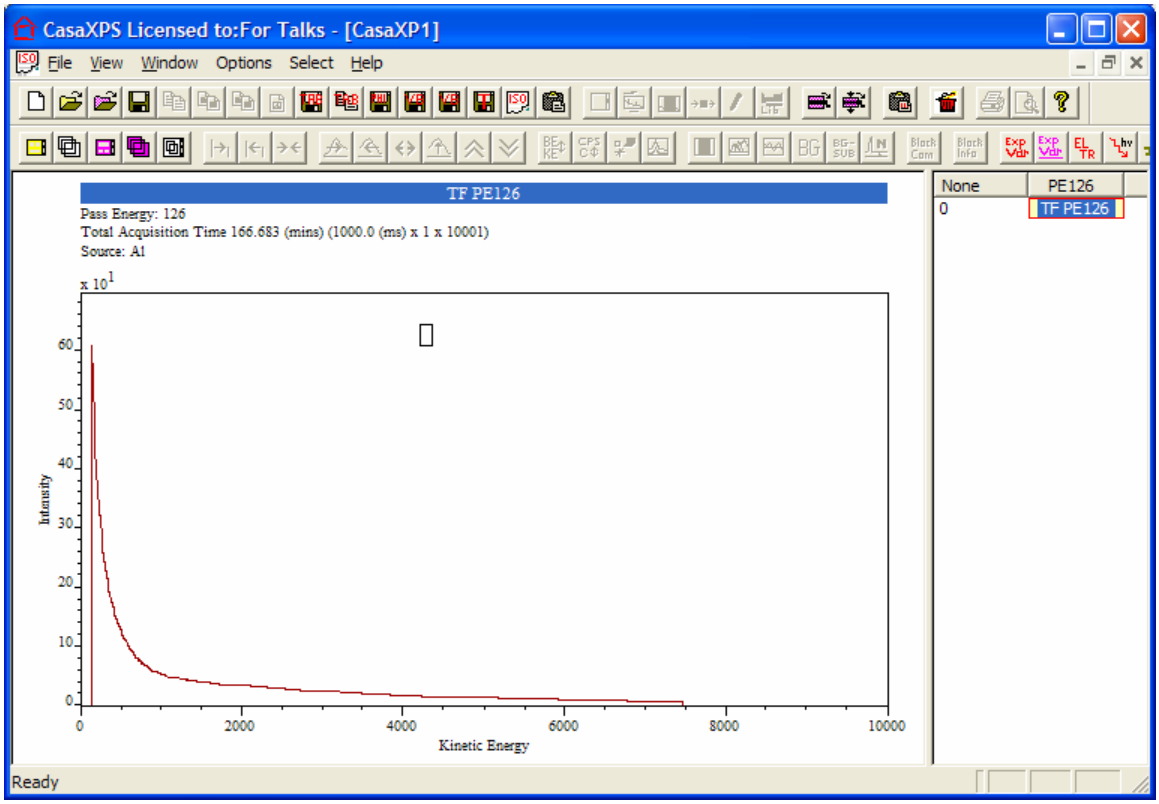
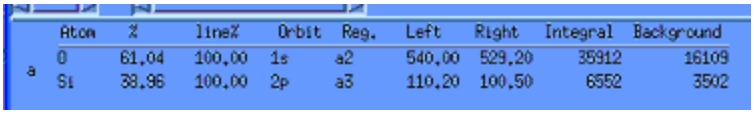


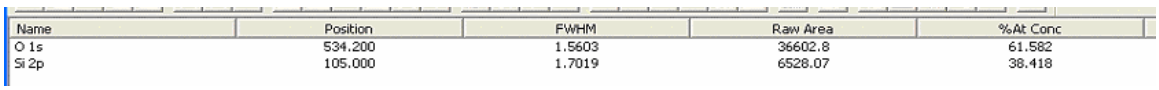
Figure 3: Transmission curve for PE 126

Quantification between SPECSLAB I and CasaXPS will be very close provided the SPECSLAB I sensitivity factors are used for both systems (Figure 4 and Figure 5).



	Aton	%	line%	Orbit	Reg.	Left	Right	Integral	Background
a	O	61,04	100,00	1s	a2	540,00	529,20	35912	16109
	Si	38,96	100,00	2p	a3	110,20	100,50	6552	3502

Figure 4: SPECLAB I PE31.5 quantification table.



Name	Position	FWHM	Raw Area	%At Conc
O 1s	534.200	1.5603	36602.8	61.582
Si 2p	105.000	1.7019	6528.07	38.418

Figure 5: CasaXPS quantification corresponding to Figure 4.