



Data analysis of Aryelle spectra and methods at ENEA

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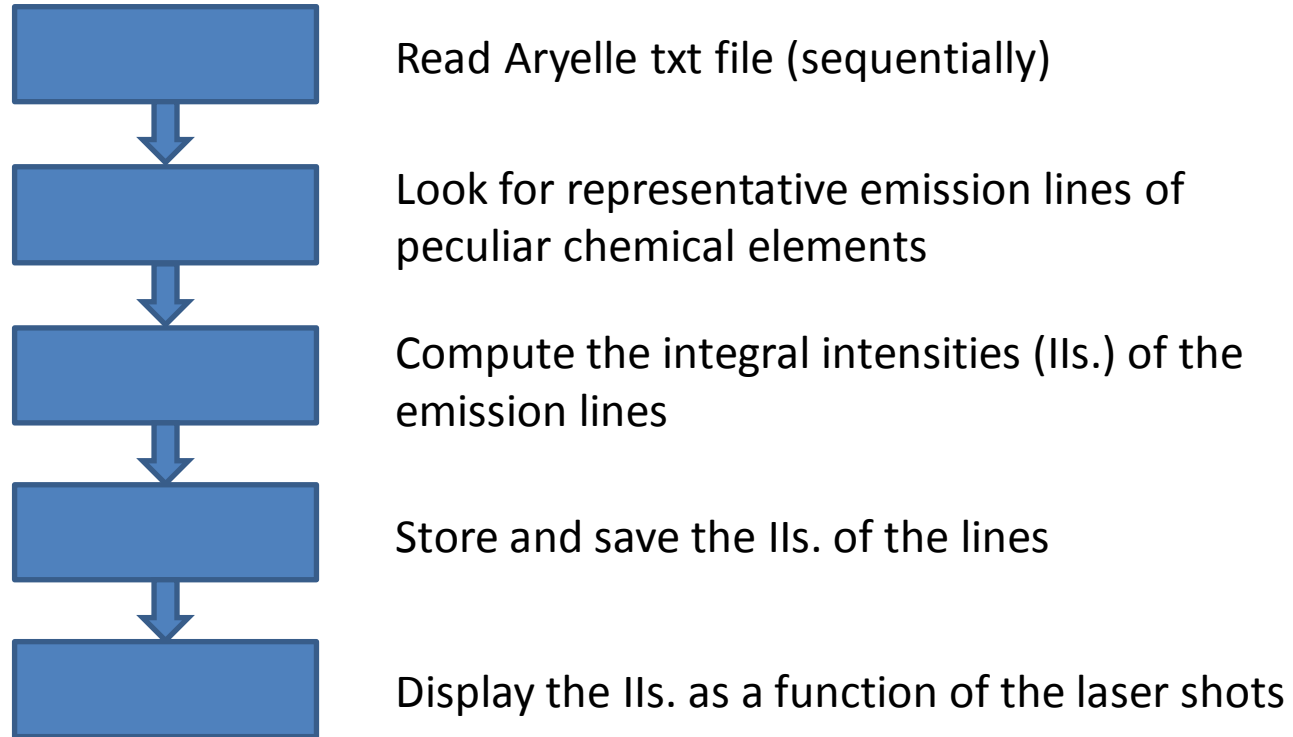
- Depth profiling data analysis of the plasma facing components (PFCs):
- Expected Results and information
- Calibration free analysis
- Expected results and information
- Conclusion



- Given the large amount of spectral data acquired during the experimental campaign «LIBS for JET», ENEA has focused the management of the data analysis through the development of scripts processing a large amount of spectral data in short time
- These scripts are developed in a MATLAB[®] environment and sequentially process the LIBS spectra acquired with the Aryelle «full range» spectrometer, preliminarily converted into '.txt' files.
- The conversion of the data from the proprietary format ('.ary') to '.txt' has been performed by using the “sophy nXt” proprietary software of the Aryelle



the operating scheme of the procedure is illustrated below:



■ Depth profiling data analysis: Matlab procedure



A MATLAB procedure has been developed to perform multiple depth profiling analyses of the acquired spectra looking at intense and free of interference emission lines of the elements.

```
tic;
clear all
d=dir('C:\Users\Almaviva-ENEA\Desktop\file_matlab_aggiornati_funzionanti'); % path to your files
l = length(d);
ind_PCA = 0;
for i =1:l
    namefile = d(i).name
    k = strfind(namefile, '.txt');
    if k >= 0
        ind_PCA = ind_PCA +1; #spectra counter
        read_Aryelle_files; peak analysis function
    end
end
delete file_appoggio.txt;
figure(3)
x_axis = linspace(1,ind_PCA,ind_PCA);
plot(x_axis,Be_I_332_11nm,'-b',x_axis,Be_I_457_27nm,'-b',x_axis,W_I_400_87nm,'-k',x_axis,W_I_407_45nm,'-k',x_axis,T_D_H_656nm,'-ro')
legend("Be I 332.11nm", "Be I 457.27nm", "W I 400.87nm", "W I 407.45nm", "T-D-H alpha 656nm", "Mo I 550.65nm", "Mo I 553.3nm", "Mo I 557.0")
xlabel('number of laser shots')
ylabel('Integral intensity (a.u.)')
figure(4)
x_axis = linspace(1,ind_PCA,ind_PCA);
semilogy(x_axis,Be_I_332_11nm,'-b',x_axis,Be_I_457_27nm,'-b',x_axis,W_I_400_87nm,'-k',x_axis,W_I_407_45nm,'-k',x_axis,T_D_H_656nm,'-ro')
legend("Be I 332.11nm", "Be I 457.27nm", "W I 400.87nm", "W I 407.45nm", "T-D-H alpha 656nm", "Mo I 550.65nm", "Mo I 553.3nm", "Mo I 557.0")
xlabel('number of laser shots')
ylabel('Integral intensity (a.u.)')
fclose all;
toc;
elapsedTime = toc;
```

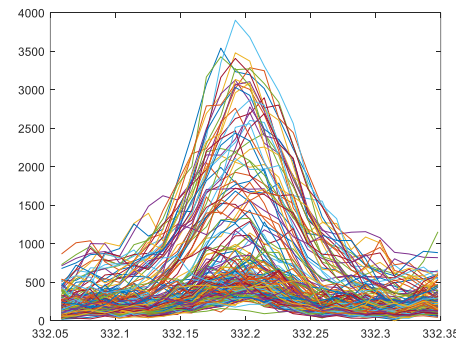
‘for’ cycle to look for ‘.txt’ files in the folder

■ Depth profiling data analysis: Matlab procedure

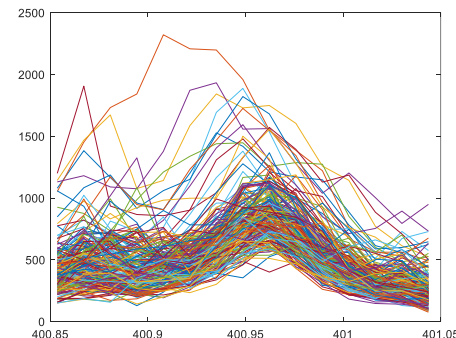


A list of the emission lines considered for each element is shown below. The rationale for choosing these lines is that they should be intense and as free from interference as possible.

Atom/Ion	Wavelength (nm)	Motivation
Be I	332.12	Be deposits on the divertor area
Be I	457.27	
W I	400.87	W substrate and redeposited material from erosion
W I	407.44	
T _α -D _α -H _α	656-656.3	Unburned (or implanted) fuel
Mo I	550.65	Mo interlayer (if present)
Mo I	553.3	
Mo I	557.04	
Cr I	425.43	Inconel structural material
Cr I	428.97	
Ni I	341.47	Inconel structural material
Ni I	345.85	
Ni I	346.16	
He I	587.58	Reaction product



Ex 1:
775_14ONG8A_R2C2
Be I line
at 332.12 nm



Ex 2:
775_14ONG8A_R2C2
W I line
at 400.87 nm



■ Depth profiling data analysis: Matlab procedure

A MATLAB procedure has been developed to perform multiple depth profiling analyses of the acquired spectra looking at intense and free of interference emission lines of the elements.

```
fin = fopen(namefile); % apre il file di input
fout = fopen('file_appoggio.txt', 'wt'); % apre il file di output di servizio non servirà alla fine
tline = fgetl(fin); % mette in tline la riga del file di input con fgetl
count = 0; %imposta a zero il contatore
while ischar(tline) % mentre il file non è finito
    tline = fgetl(fin); % metti in tline la riga del file di input con fgetl
    if tline ~= -1 % questa istruzione perchè alla fine di ogni file mette un "-1"
        fprintf(fout, '%s\n', tline); %scrivi come riga sul file di output
        count = count + 1;
    end
end
fclose(fout); % chiudi l'output
load file_appoggio.txt %ricarica il file di servizio
x = file_appoggio(:,1); %colonna delle lunghezze d'onda
y = file_appoggio(:,2);
```

```
indices = find( x > 341.38 & x <= 341.58);
Ni_I_341_48nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 345.75 & x <= 345.95);
Ni_I_345_85nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 346.065 & x <= 346.265);
Ni_I_346_165nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 400.83 & x <= 400.94);
W_I_400_87nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 407.35 & x <= 407.55);
W_I_407_45nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 425.34 & x <= 425.54);
Cr_I_425_44nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 427.38 & x <= 427.58);
Cr_I_427_48nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 428.9 & x <= 429.1);
Cr_I_429_00nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 332 & x <= 332.35);
figure(1)
plot(file_appoggio(min(indices):max(indices),1),file_appoggio(min(indices):max(indices),2))
hold on
Be_I_332_11nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 457.24 & x <= 457.43);
Be_I_457_27nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 550.55 & x <= 550.75);
Mo_I_550_65nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 553.2 & x <= 553.4);
Mo_I_553_3nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 556.94 & x <= 557.14);
Mo_I_557_04nm(ind_PCA,1) = sum(y(min(indices): max(indices)));
indices = find( x > 587.49 & x <= 587.69);
```

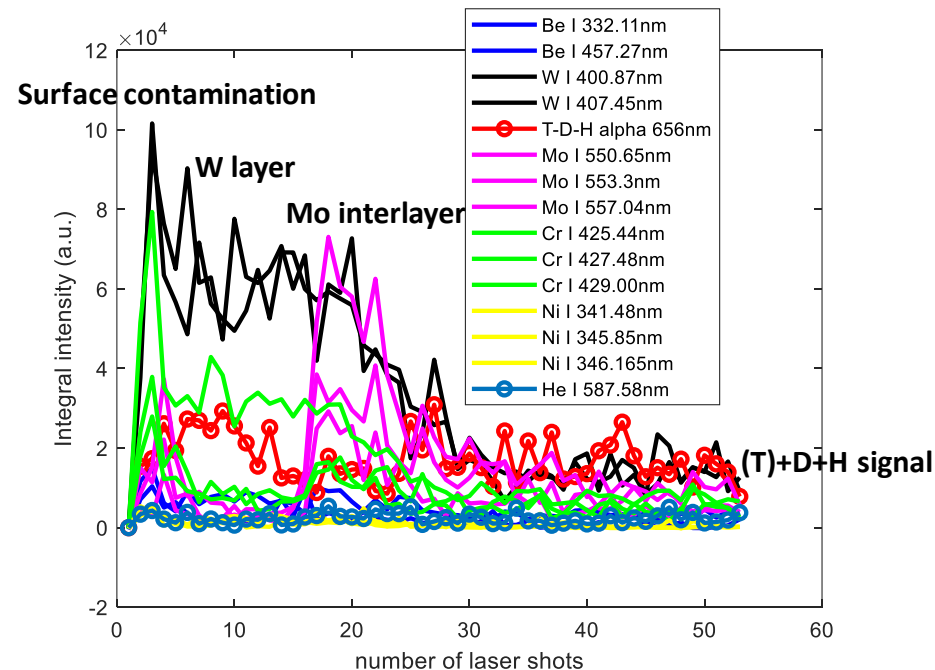
Look for Ni I @ 341.48 nm...

Look for W I @ 400.87 nm...

Look for Be I @ 332.11 nm...

Look for Mo I @ 550.65 nm...

Ex. WEST sample C3-34-iK (VTT campaign in March 2024)

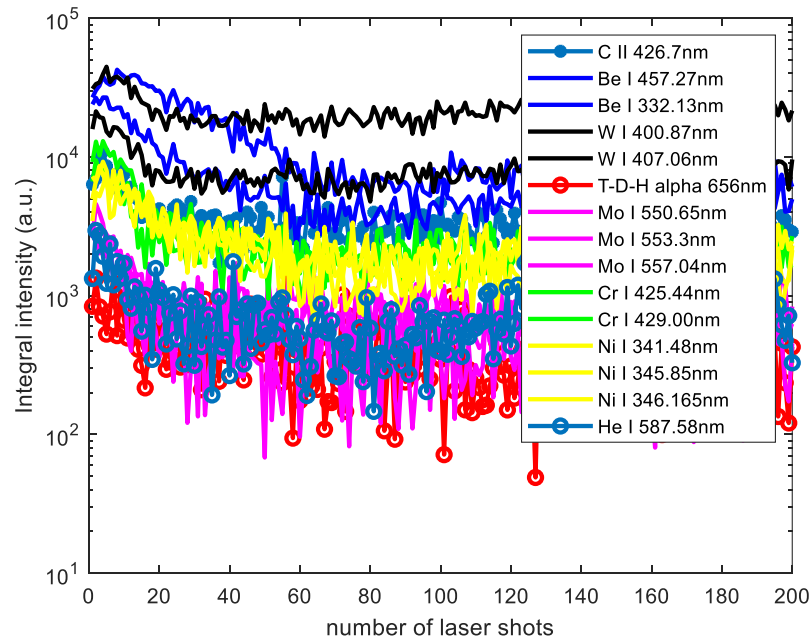
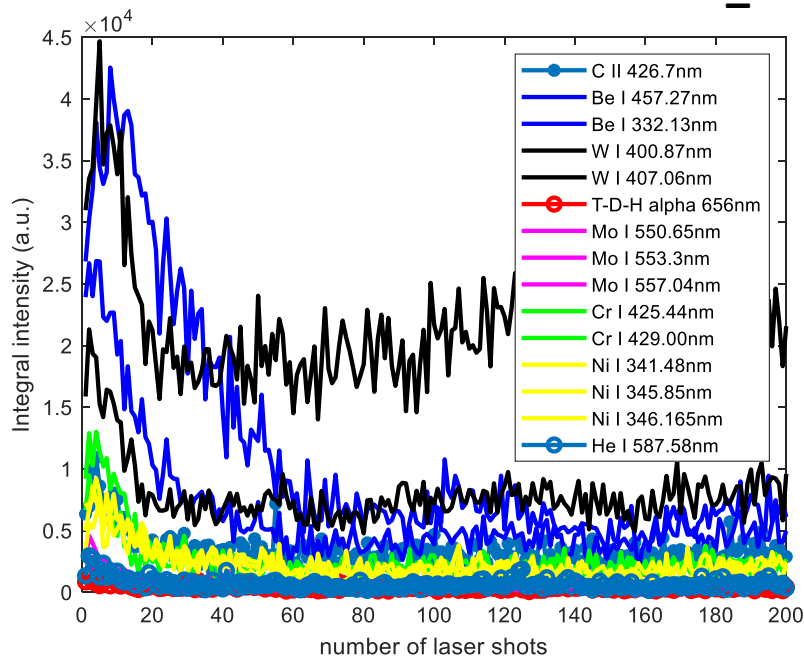


■ Depth profiling data analysis: Matlab procedure



The entire output is displayed in two graphs showing line intensities as a function of laser shots, both with linear and semi-logarithmic scales. Graph can be saved in common graph formats (e.g. .tiff or .jpeg) and data in .txt format for further analyses or processing.

775_14ONG8A_R2C2



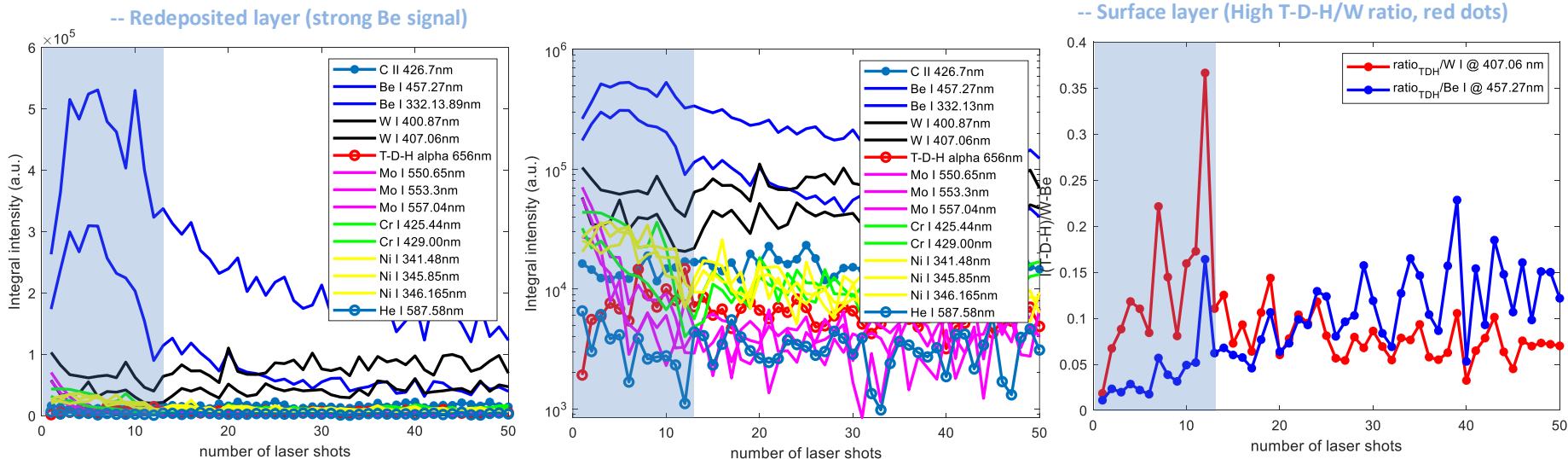
■ Depth profiling data analysis: Expected Results and information



With these procedures the following information on the PFCs of the divertor can be obtained:

- 1) thickness of the layer of redeposited material as a function of the applied laser shots along the whole divertor profile
- 2) Presence of unburned fuel (T+D) and its distribution in-depth
- 3) possible traces of eroded structural materials (mainly Ni and Cr from Inconel steel)
- 4) Intensity ratio T+D+H/W for qualitative in-depth distribution of T+D+H

Ex: LIBS at JET. Point 59_HFGC_LH14W_R1C1





■ Depth profiling data analysis: Matlab procedure

The procedure takes a few seconds per spectrum to complete, the processing time depending on the performance of the PC used. Ex. this PC (CPU intel core i5, RAM 8 GB) = **293.5 sec for 200 spectra**

The screenshot displays the MATLAB R2023b environment. The **EDITOR** tab is active, showing a script named `load_multiple_files_Aryelle_LIBS.m`. The script performs the following steps:

- 1. `tic;` (Starts timing)
- 2. `clear all` (Clears workspace)
- 3. `d=dir('C:\Users\Salvatore Almagiva\Desktop\file_matlab_aggiornati_funzionanti'); % path to your files` (Gets directory listing)
- 4. `l = length(d);` (Gets number of files)
- 5. `ind_PCA = 0;` (Initializes PCA index)
- 6. `for i =1:l` (Starts loop over files)
- 7. `namefile = d(i).name` (Gets filename)
- 8. `k = strfind(namefile, '.txt');` (Finds .txt extension)
- 9. `if k >= 0` (Checks for .txt)
- 10. `ind_PCA = ind_PCA +1;` (Increments PCA index)
- 11. `read_Aryelle_files;` (Calls function to read files)
- 12. `end` (Ends if loop)
- 13. `end` (Ends for loop)
- 14. `delete file_appoggio.txt;` (Deletes temporary file)
- 15. `figure(7)` (Opens figure window)
- 16. `x_axis = linspace(1,ind_PCA,ind_PCA);` (Creates x-axis for plot)
- 17. `plot(x_axis,C_I_426_7nm, '-*',x_axis,Be_I_457_27nm, '-b',x_axis,Be_I_332_13nm, '-b',x_axis,W_I_400_87nm` (Plots multiple data series)
- 18. `legend('C II 426.7nm', 'Be I 457.27nm', 'Be I 332.13nm', 'W I 400.87nm', 'W I 407.06nm', 'T-D-H alpha 656` (Adds legend)
- 19. `xlabel('number of laser shots')` (Sets x-axis label)
- 20. `ylabel('Integral intensity (a.u.)')` (Sets y-axis label)
- 21. `figure(8)` (Opens another figure window)
- 22. `save('save.mat', 'ind_PCA', 'ind_PCA');` (Saves variables)

The **Workspace** window on the right shows the following variables:

Name	Value
ans	0
Be_I_332_13nm	200x1 double
Be_I_457_27nm	200x1 double
C_II_426_7nm	200x1 double
count	40306
Cr_I_425_44nm	200x1 double
Cr_I_428_97nm	200x1 double
d	224x1 struct
elapsedTime	293.5422
file_appoggio	40306x2 double
fin	202
fout	203
He_I_587_49nm	200x1 double
i	224
ind_PCA	200
indices	14x1 double
k	[]
l	224
Mo_I_550_65nm	200x1 double
Mo_I_553_3nm	200x1 double
Mo_I_557_04nm	200x1 double
namefile	'subtract_background_Aryelle.m'
Ni_I_310_16nm	200x1 double
Ni_I_338_06nm	200x1 double
Ni_I_341_48nm	200x1 double
T_D_H_656nm	200x1 double
tline	-1
W_I_400_87nm	200x1 double
W_I_407_06nm	200x1 double
x	40306x1 double
x_axis	1x200 double
y	40306x1 double

The **Command Window** at the bottom shows the execution progress and the final elapsed time:

```
New to MATLAB? See resources for Getting Started.  
'smoothing_multiplo_Aryelle.m'  
  
namefile =  
  
'subtract_background_Aryelle.m'  
  
Elapsed time is 293.532190 seconds.  
fx >>
```

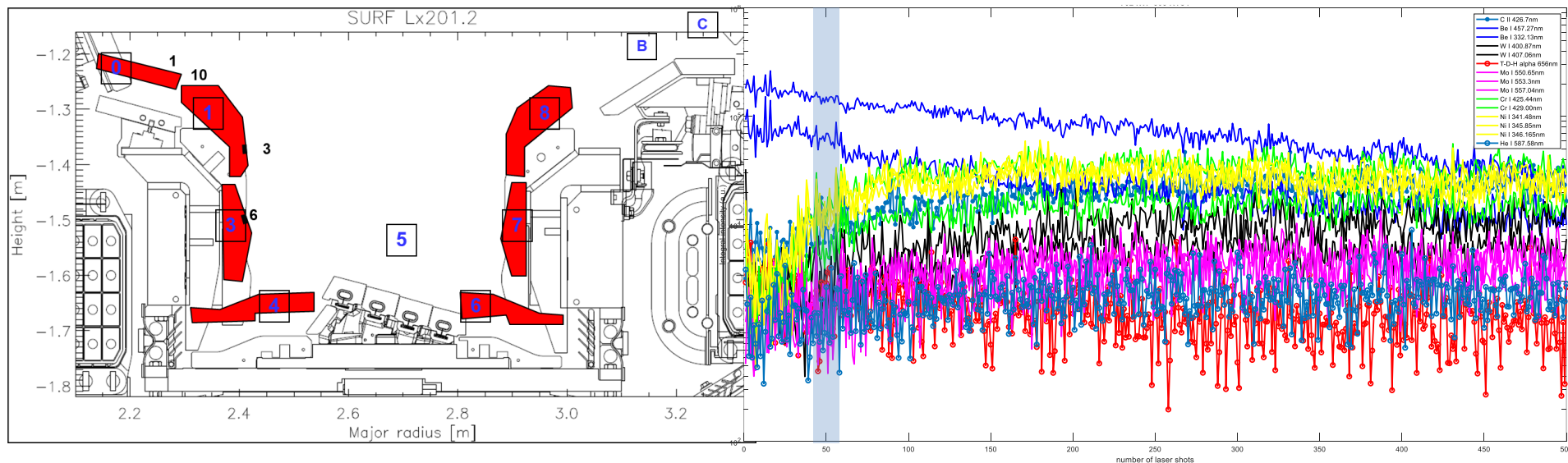
Outputs:
(in light blue)
IIs of the emission
Lines as a function of
The applied laser shots

■ Depth profiling data analysis: Expected Results and information



The information obtained concerns the presence and thickness (preliminarily in terms of laser shots) of the layers deposited on the surface of the divertor PFCs, the in-depth distribution of nuclear fuel and any erosion phenomena of the PFCs.

The average ablation rate for Be has been estimated on point 702_IWP_808_R1C1: 8 μm Be coating on Inconel steel $\approx$ 50 shot $\rightarrow$ AAR 160 nm per shot



■ Calibration free analysis: Matlab procedure



The CF procedure (Appl. Spec. 53(8), (1999), 960-964) aims to quantitatively estimate the chemical elements detected in the LIBS plasma. CF will be applied to estimate the concentration of T+D+H (the latter being present as residual impurity in the spectrum) respect to W (bulk material of the divertor PFCs) and respect to Be (bulk material of the first wall and major eroded material on the divertor PFCs).

CF is based on the experimental intensities of the emission lines.

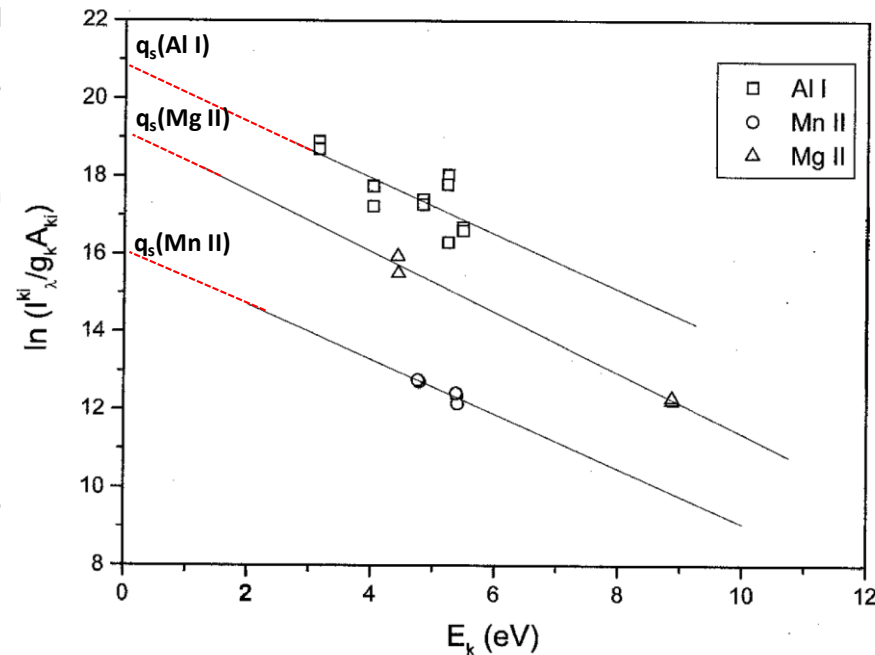
Indeed, if the LIBS plasma can be considered in local thermodynamic equilibrium (LTE) these intensities can be expressed as follows:

$$I_{\lambda}^{ki} = C_s A_{ki} \frac{g_k e^{-(E_k/k_B T)}}{U_s(T)}$$

where, I_{λ}^{ki} = exp. intensity of the $k \rightarrow i$ transition, C_s = concentration of the species, A_{ki} = transition probability for the given line, g_k is the k level degeneracy, E_k the upper energy level of the transition, k_B^T = Boltzmann constant, $U_s(T)$ is the partition function for the emitting species at the plasma temperature T_e .

The emission lines of each species can be plotted as points in a graph (**Boltzmann plot, BP**) and their linear fits give an intercept, q_s which is related to the relative concentration of the species through the following equation:

$$C_s = \frac{U_s(T_e)}{F} e^{q_s}$$



(Appl. Spec. 53(8), (1999), 960-964)



■ Calibration free analysis & Matlab procedure: compute T_e

To apply the CF procedure it is necessary to consider the atomic and ionic emission lines of each element under analysis, complete of their spectroscopic parameters and the partition function of the emitting species at the plasma temperature; this was done for W I, W II, Be I, Be II, H(D,T), the data being retrieved from the NIST website (<https://www.nist.gov/pml/atomic-spectra-database>). Below **(left)** an example of the data for W I and **(right)** the partition functions of W I and H at typical temperatures of the LIBS plasmas.

Observed Wavelength Air (nm)	A_{ki} (10^8 s^{-1})	Acc.	E_i (eV)	E_j (eV)	$g_i - g_k$
400.1380	5.6e-03	B	1.507891	4.605562	9 - 9
400.87506	1.63e-01	B	0.365913	3.457888	7 - 9
401.9227	6.7e-03	B	0.412313	3.496218	5 - 3
402.8786	2.48e-02	B	1.181329	4.257920	1 - 3
403.5356	2.90e-02	B	1.916797	4.988377	7 - 9
403.6855	1.49e-01	B	2.387469	5.457908	9 - 7
404.3894	1.42e-01	C	2.387137	5.452232	5 - 5
404.5594	2.88e-02	B	0.365913	3.429715	7 - 5
404.7938	5.00e-04	C	0.207090	3.269126	3 - 5
405.3932	4.9e-02	B	1.856810	4.914315	5 - 3
405.523	1.79e-03	C	1.655011	4.711538	7 - 9
406.0705	5.9e-02	B	2.458319	5.510728	7 - 7
406.4791	1.59e-01	B	2.387469	5.436811	9 - 7
406.9950	3.60e-02	B	0.598844	3.644317	7 - 5
407.0608	5.7e-03	B	0.207090	3.252077	3 - 5
407.1928	3.29e-02	B	1.916797	4.960794	7 - 5
407.4358	1.0e-01	B	0.365913	3.408091	7 - 7
408.8330	4.13e-03	C	0.412313	3.444095	5 - 3
410.2702	4.9e-02	B	0.771099	3.792268	9 - 7
410.2942	4.2e-04	C	0.598844	3.619823	7 - 5

NIST data

File	Modifica	Visualizza
4001.380	4.6056	9
4008.751	3.4579	9
4019.227	3.4962	3
4028.786	4.2579	3
4035.356	4.9884	9
4036.855	5.4579	7
4043.894	5.4522	5
4045.594	3.4297	5
4047.938	3.2691	5
4053.932	4.9143	3
4055.230	4.7115	9
4060.705	5.5107	7
4064.791	5.4368	7
4069.950	3.6443	5
4070.608	3.2521	5
4071.928	4.9608	5
4074.358	3.4081	7
4088.330	3.4441	3
4102.702	3.7923	7
4102.942	3.6198	5

wv (Å)

E_k (eV) g_k

E_i (eV) g_i

A_{ki} (10^8 s^{-1})

File	Modifica	Visualizza	File	Modifica	Visualizza
6962.715003702	21.92	2	6962.715003702	2	
7542.941254010	24.46	2	7542.941254010	2	
8123.167504319	29.44	2	8123.167504319	2	
8703.393754627	33.91	2	8703.393754627	2	
9283.620004936	38.9	2	9283.620004936	2	
9863.846255244	44.43	2.01	9863.846255244	2.01	
10444.07250555	50.51	2.01	10444.07250555	2.01	
11024.29875586	57.17	2.03	11024.29875586	2.03	
11604.52500617	64.4	2.06	11604.52500617	2.06	
12184.75125647	72.21	2.11	12184.75125647	2.11	
12764.97750678	80.61	2.19	12764.97750678	2.19	
13345.20375709	89.58	2.33	13345.20375709	2.33	
13925.43000740	99.12	2.54	13925.43000740	2.54	
14505.65625771	109.22	2.85	14505.65625771	2.85	
15085.88250802	119.86	3.3	15085.88250802	3.3	
15666.10875832	131.03	3.91	15666.10875832	3.91	
16246.33500863	142.7	4.73	16246.33500863	4.73	
16826.56125894	154.85	5.81	16826.56125894	5.81	
17406.78750925	167.47	7.21	17406.78750925	7.21	
17987.01375956	180.53	8.97	17987.01375956	8.97	
18567.24000987	194	11.17	18567.24000987	11.17	
19147.46626018	207.86	13.85	19147.46626018	13.85	
19727.69251048	222.09	17.1	19727.69251048	17.1	

T (K)

U(T)

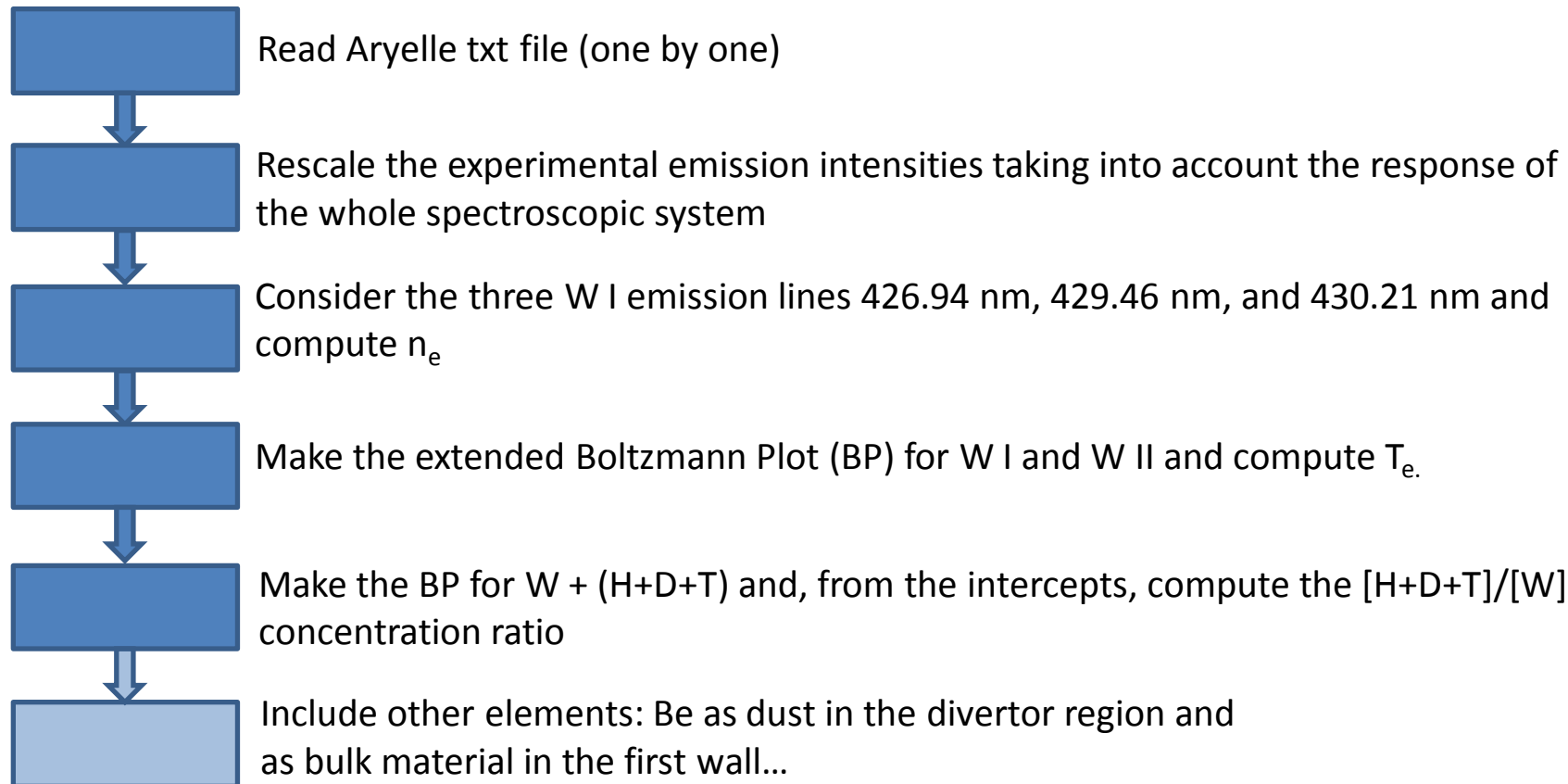
T (K)

U(T)

- Calibration free analysis & Matlab procedure: rescale the experimental intensities



the operating scheme of the procedure is illustrated below:



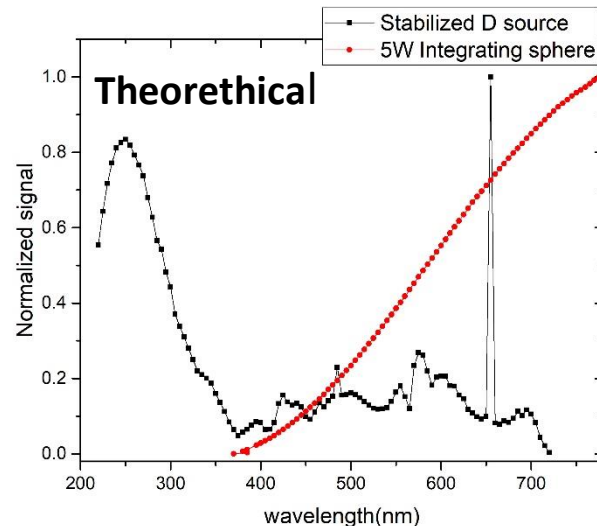
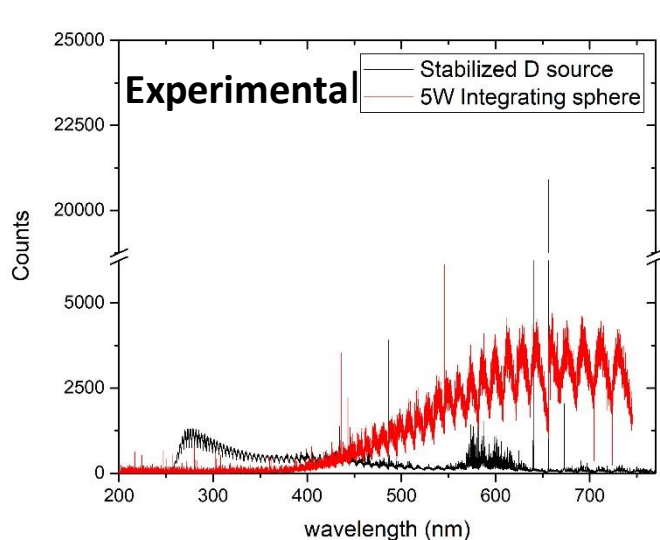
- Calibration free analysis & Matlab procedure: rescale the experimental intensities



Two preliminary steps have been applied to the raw data to make them suitable for CF:

1. Rescaling the intensity of the emission lines through the spectra of the D lamp and the Integrating sphere (intensity calibration)
2. Subtraction of the background signal induced by the spectrometer orders (background subtraction)

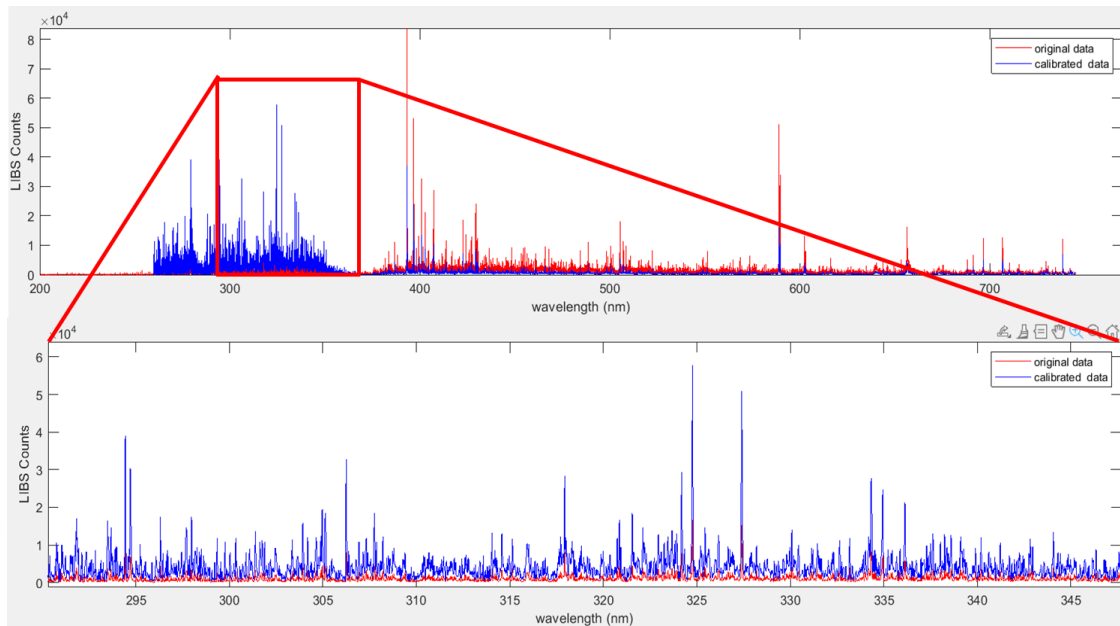
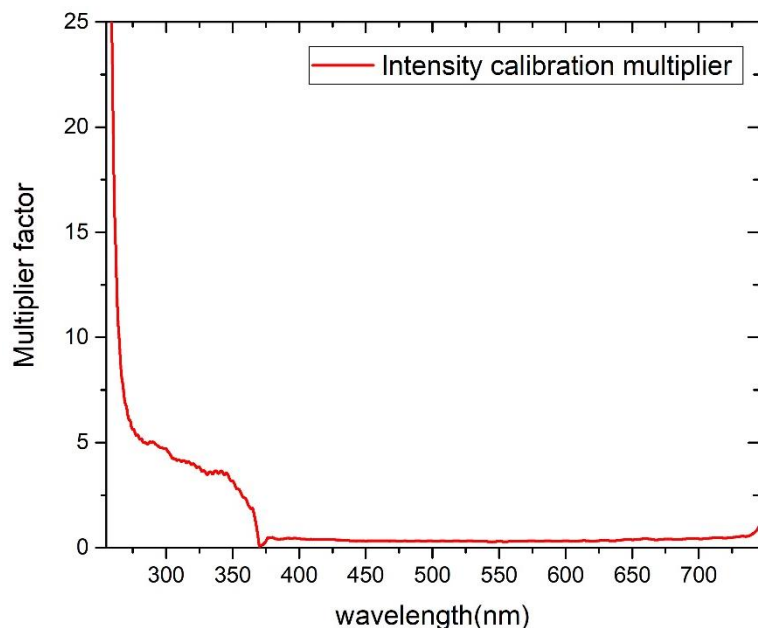
The intensity calibration was obtained by comparing the reference spectral signal of the stabilized deuterium UV light source and the 5W integrating sphere with that obtained by the Aryelle spectrometer.



- Calibration free analysis & Matlab procedure: rescale the experimental intensities



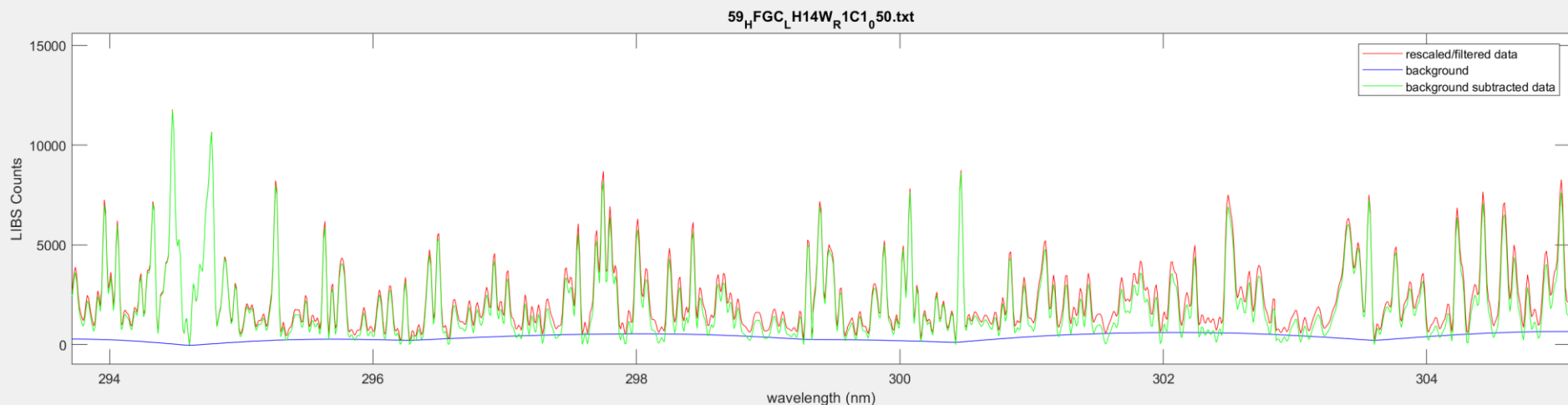
After the comparison, a calibration file, containing multiplication factors as a function of the wavelength was obtained for the region from 260 to 370 to rescale the experimental intensity with that theoretical of the deuterium lamp and from 370 to 740 nm to rescale the experimental intensity with that theoretical of the 5W integrating sphere.



- Calibration free analysis & Matlab procedure: rescale the experimental intensities



The background subtraction was obtained by applying an iterative smoothing procedure with a moving average filter (3 close points) to the original data in order to suppress the peaks and obtain a smoothed background to subtract to the original data. The net result is a full range spectrum without any additional background signal from the sequence of the spectrometer's orders, as shown as an example in the following figure:



- Calibration free analysis & Matlab procedure: compute n_e



To make the BP of each chemical species more reliable to obtain it is a common procedure to make the extended BP, where atoms and ions are displayed together in the same BP, once the coordinates of the ions are modified as follows:



Spectrochimica Acta Part B 62 (2007) 378–385



$$E_{k-ions} = E_{k \rightarrow i} + E_{ionization}$$

$$\ln \left(\frac{I_{k \rightarrow i}}{g_k A_{k \rightarrow i}} \right)_{ions} = \ln \left(\frac{I_{k \rightarrow i}}{g_k A_{k \rightarrow i}} \right) - \ln \left[2 \left(\frac{mk}{2\pi\hbar^2} \right)^{\frac{3}{2}} \frac{T^{\frac{3}{2}}}{n_e} \right]$$

therefore, the electron density, n_e is the needed parameter to include ions in the BP of the species.

Through the knowledge of n_e it is also possible to have the relative concentration of atoms and ions of the same chemical species through the **Saha-Boltzmann equation**:

$$\frac{C_{ions}}{C_{atoms}} = \frac{2U_{ions}(T_e)}{n_e U_{atoms}(T_e)} \left(\frac{mk_B T}{2\pi\hbar^2} \right) e^{-\frac{E_{ion}}{k_B T}}$$

(E_{ion} = ionization energy, m = electron mass)

necessary to correctly quantify the concentrations of the chemical species

Multi-element Saha–Boltzmann and Boltzmann plots in laser-induced plasmas

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$$\ln \left(\frac{\varepsilon^z \lambda}{A g_j} \right)^* = \ln \left(\frac{\varepsilon^z \lambda}{A g_j} \right) - B^z(T, N_e) \quad (2)$$

where

$$B^z(T, N_e) = z \ln \left[2 \left(\frac{mk}{2\pi\hbar^2} \right)^{3/2} \frac{T^{3/2}}{N_e} \right] \quad (3)$$

and

$$E_j^{z*} = E_j^z + \sum_{k=0}^{z-1} (E_{\infty}^k - \Delta E_{\infty}^k) \quad (4)$$

*Spectrochim. Acta B 62 (2007) 378–385

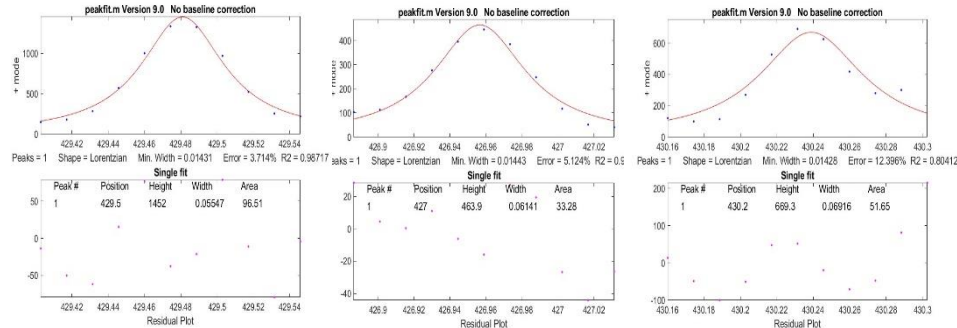


■ Calibration free analysis & Matlab procedure: compute n_e

The electron density was computed according to the following formula:

$$n_e = \frac{\Delta\lambda_{FWHM}}{w_{FWHM}^0} (10^{23} \text{m}^{-3})$$

where $\Delta\lambda_{FWHM}$ is the experimental line broadening (reduced by the instrumental broadening which was estimated through the emission lines of the low pressure Hg lamp)



and w_{FWHM}^0 is the Stark parameter of the three W I lines at 426.9, 429.4, 430.2 nm from the Nishijima and Doerner publication (J. Phys. D: Appl. Phys. 48 (2015) 325201 (6pp)):

Table 1. Summary of W I Stark FWHM.

λ (nm)	T_e (eV)	n_e (10^{23}m^{-3})	w_{FWHM} (nm)	w_{FWHM}^0 at 10^{23}m^{-3} (nm)
426.9	0.73–0.99	0.12–0.41	0.00940–0.0248	0.0634 ± 0.0022
429.4	0.73–1.0	0.12–0.41	0.00727–0.0226	0.0513 ± 0.0022
430.2	0.83–0.99	0.19–0.41	0.00537–0.0157	0.0330 ± 0.0026

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Stark width measurements and Boltzmann plots of W I in nanosecond laser-induced plasmas

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Abstract

We report the first measurements of Stark broadening widths of W I lines (426.9 nm, 429.4 nm, and 430.2 nm) as a function of electron density, n_e . The electron density is obtained from Stark broadening of a C II line at 426.7 nm in nanosecond laser-induced tungsten carbide plasmas. A linear relation between the W I Stark widths and n_e is confirmed. The electron temperature, T_e , is evaluated from Boltzmann plots of W I transitions with an oscillator strength $f_{ik} < 1.0 \times 10^{-2}$, since systematically lower population densities are observed for W I transitions with $f_{ik} \geq 1.0 \times 10^{-2}$, indicating that absorption occurs. This is consistent with an overestimated n_e derived from Stark broadening of the 429.4 nm line ($f_{ik} = 2.45 \times 10^{-2}$) at a high ambient gas pressure.

Keywords: W I Stark width, W I Boltzmann plot, laser-induced plasma

(Some figures may appear in colour only in the online journal)



Calibration free analysis & Matlab procedure: compute T_e

Searching in the database accessible by the procedure, the experimental spectrum is compared with the theoretical one and if the spectral distance between experimental and theoretical lines is below a certain threshold (typically 50 pm) the lines are identified. Using these lines the extended BP for W (and, in the next steps, for Be) can be setup.

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load_multiple_files_Aryelle.m  make_BP.m  make_ext_BP.m  calibration_free.m  subtract_background_Aryelle.m  peakfit_test.m  +

1  z = 1;
2  for i = 1:l_locs
3      for s = 1:l_DB
4          diff = abs(locs(i,1) - W_tot(s,1));
5          if diff < 0.05
6              peaks(z,1) = locs(i,1);
7              peaks(z,2) = W_tot(s,1);
8              peaks(z,3) = diff;
9              peaks(z,4) = pks(i,1)*w(i,1)*1.064467; %approx of a gaussian area given the peak max and the FWHM
10             peaks(z,5) = W_tot(s,3)*W_tot(s,6); %gk*Ak
11             switch W_tot(s,9)
12                 case {1}
13                     peaks(z,6) = W_tot(s,2);
14                     peaks(z,7) = log((peaks(z,4)*peaks(z,2))/(peaks(z,5)));
15                     peaks(z,8) = 1;
16                 case {4, 4.5}
17                     if W_tot(s,9) == 4.5
18                         peaks(z,6) = W_tot(s,2) + 9.322699;
19                         peaks(z,7) = log((peaks(z,4)*peaks(z,2))/(peaks(z,5)))-log(((1.4e-78)*(T_e^1.5))/((2.91e-100)*(n_e)));
20                         peaks(z,8) = 4.5;
21                     else
22                         peaks(z,6) = W_tot(s,2);
23                         peaks(z,7) = log((peaks(z,4)*peaks(z,2))/(peaks(z,5)));
24                         peaks(z,8) = 4;
25                     end
26                 case {74, 74.5}
27                     if W_tot(s,9) == 74.5
28                         peaks(z,6) = W_tot(s,2) + 7.86403;
29                         peaks(z,7) = log((peaks(z,4)*peaks(z,2))/(peaks(z,5)))-log(((1.4e-78)*(T_e^1.5))/((2.91e-100)*(n_e)));
30                         peaks(z,8) = 4.5;
31                     else
32                         peaks(z,6) = W_tot(s,2);
33                         peaks(z,7) = log((peaks(z,4)*peaks(z,2))/(peaks(z,5)));
34                         peaks(z,8) = 74;
35                     end
36             end
37         end
38     end
39     z = z+1;
40 end

```

H-D-T

Be I

Be II

W I

W II

routines for Be (atom and ions)

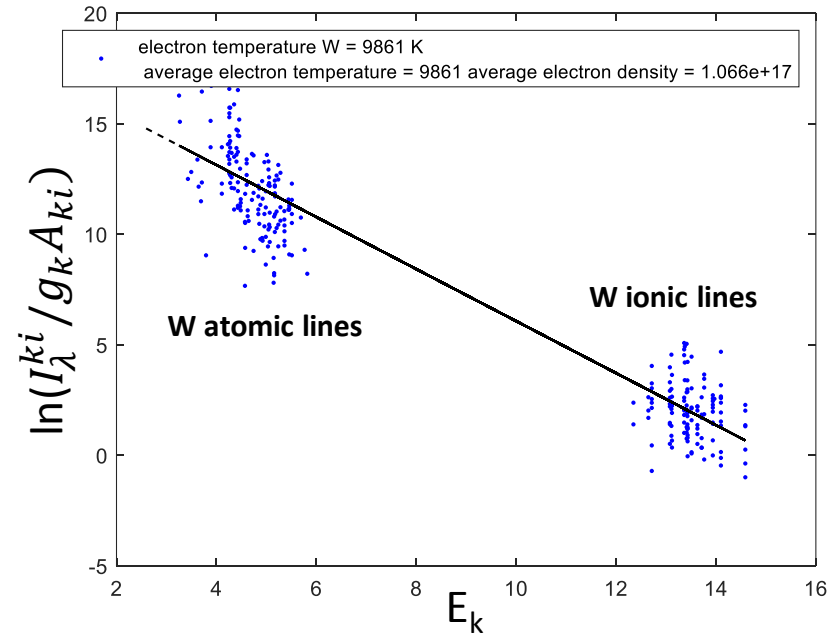
routines for W (atoms and ions)

Evaluate the spectral distance

Assign E_k

Compute $\ln(I_{\lambda}^{ki}/g_k A_{ki})$

Prepare data for H-D-T ($z = 1$)



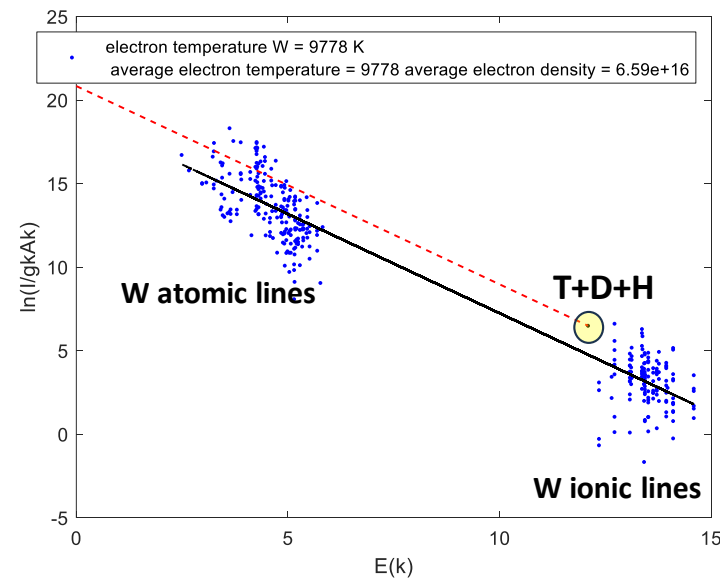
- Calibration free analysis & Matlab procedure: evaluate $[T+D+H]/[W]$



Once the Extended BP for W is setup, the sum of the spectral signal of the Balmer alpha emission T_α , D_α , H_α is included in the BP because the Aryelle spectrometer cannot spectrally resolve the three emission lines but consider the T+D+H signal as a single spectral emission. By applying CF the relative concentration $[T+D+H]/[W]$ is obtained and rescaled in percentage.

Line	wv(nm)	E_i (eV)	E_k (eV)	$g_k A_{ki}(s^{-1})$
T_α	656.047	10.2	12.09	3.88
D_α	656.107	10.2	12.09	3.88
H_α	656.285	10.2	12.09	3.88

* Data taken from NIST

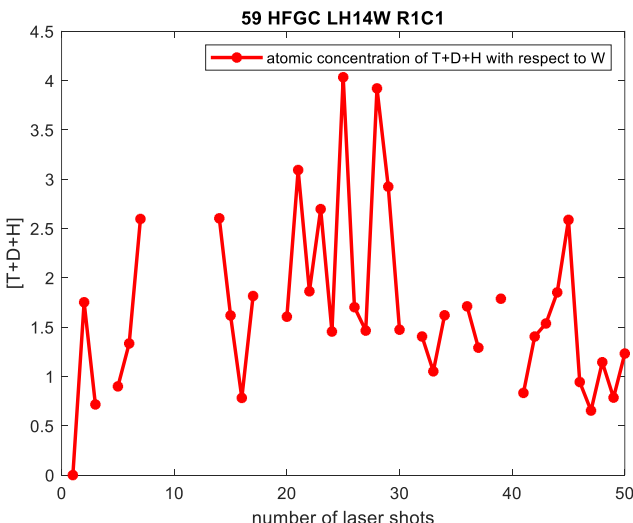
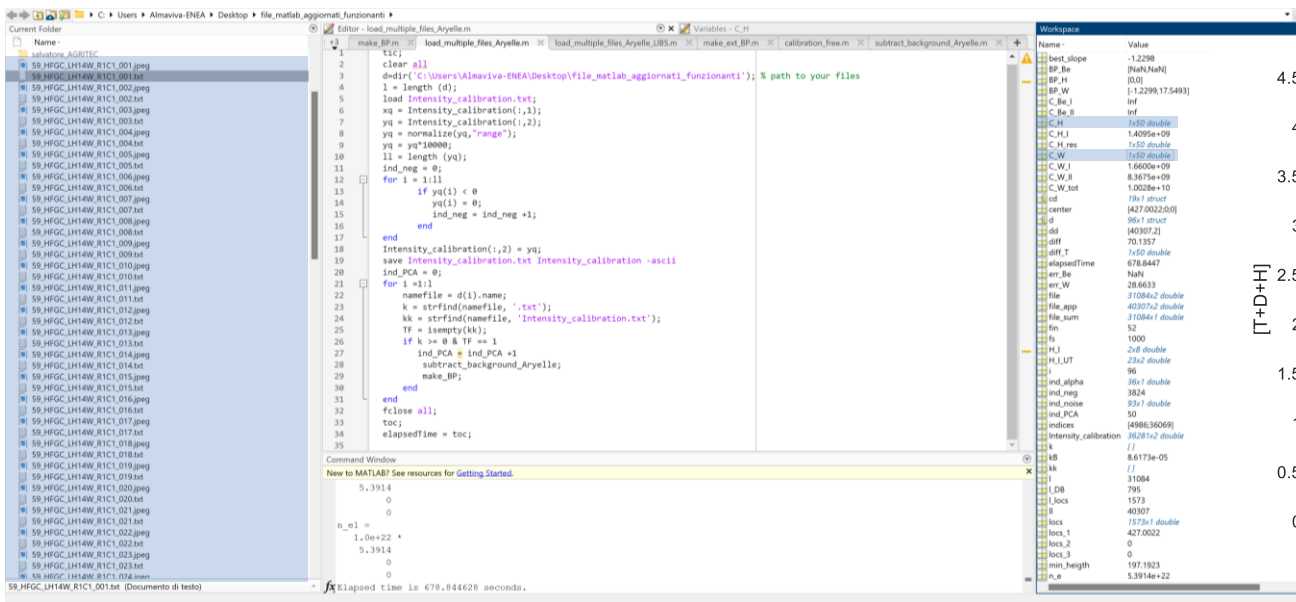


Calibration free analysis & Matlab procedure : Expected Results and information



With these procedures the following information on the PFCs of the divertor can be obtained:

- 1) Atomic concentration (%) of T+D+H with respect to W (bulk material)
- 2) (ongoing) Atomic concentration (%) of T+D+H with respect to Be (redeposited material)
- 3) In-depth atomic concentration (%) of T+D+H with respect to W (bulk material) and Be (ongoing)
- 4) Electron temperature and electron density of the LIBS plasma
- 5) Estimated processing time (currently): ≈ 15 sec per spectrum





- 1) The automatic procedure we are going to implement allows to process large amounts of spectral data in relatively short times
- 2) The development of such routines has focused on obtaining two main information:
 - 1) The qualitative in-depth distribution (as a function of the applied laser shots) of the main chemical elements of interest, with particular attention to T+D(+H), H being present as a residue of environmental contamination
 - 2) The concentration of T+D(+H) with respect to tungsten, considered as bulk material of the divertor PFCs
- 3) The further development of the scripts is planned to include in the processing also Be, as bulk material of the first wall and obtain data for the concentration of T+D(+H), in PFCs of the first wall.