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Development of a Simple Software Program Used for Evaluation of Plasma Electron Density in LIBS Experiments via Spectral Line Shape Analysis

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ABSTRACT

A Software program has been developed in order to perform a fast and reliable calculation to plasma electron density in laser induced breakdown spectroscopy (LIBS) experiments. This program is based on analyzing the emitted spectral line shape via utilizing facilities of the MatLab7® package to perform this task. This software can perform the following tasks; read the exported data file (*txt-format) from ICCD camera-software, specify the working wavelength of interest, removes the continuum emission component appeared under the line, calculates the spectral line intensity of the line, calculates the spectral shift of the line from the tabulated values, correct against spectral shift jitter at the peak emission, de-convoluting and extracting the different components contributing to the emitted line full width at half of the maximum (FWHM) and finally calculates the plasma electron density. In this article we shall present the results of the test measurement of the plasma electron density utilizing spectral line shape analysis to the emitted H_α-line, Si I-line at 288.15 nm and O I-line at 777.2 nm at different camera delay times ranging from 1 to 5 µs.

Keywords: Software; LIBS; H_α-Line; Electron Density; MatLab7®

1. Introduction

LIBS, is an acronym derived from the letter words of the statement "Laser Induced Breakdown Spectroscopy"[1]. It is a technique based on utilizing light emitted from plasma generated via interaction of a high power lasers with matter (solid, liquid or gases). Assuming that light emitted is sufficiently influenced by the characteristic parameters of the plasma, the analysis of this light yields considerable information about the elemental structure and the basic physical processes in plasma [2]. The thermodynamic state of plasma can be identified via two independent measurable parameters namely; electron density and temperature [2]. In the passive optical emission spectroscopy (OES) mode, light analyzers (spectrographs or monochromators) with a graphical readout are employed to give the characteristic emission spectrum. A spectrum is the functional dependence of the output light spectral intensity (radiance) on the emission wavelength [3-5].

Among the OES methods proposed for the measurement electron density, the spectral broadening of emission lines due to the Stark effect is the most widely use method [3]. This method is based on the assumption that the Stark effect is the dominant broadening mechanism, in comparison to the Doppler and other broadening mechanisms (resonance and Van der Waals broadenings). The validity of this assumption was generally admitted in LIBS experiments and was justified in various studies [6].

Over the tremendous number of the recorded spectra under a variety of different experimental conditions, the extraction of the information's from spectra provides a strong motivation to a fast and precise computer routine for calculation of plasma parameters. This information's are generally stored in the spectral line width (FWHM) and the signal height (spectral radiance). The FWHM is a sensitive function of the Stark and other broadening mechanism, while the spectral radiance is sensitive to plasma temperature and/or elemental concentration [7].

A computer programming used for spectral line shape analysis is not new, several authors have contributed by their work in this field, but the exact processing method were almost not clear which might lead to confusion [8-10]. Several software simulation programs based on different theories were developed to calculate the electron density from the FWHM of the hydrogen lines at the

Balmer series [11,12].

In this article we will present the results of using a straight forward computer routine written in Matlab7® package used for fast and reliable calculation of the plasma electron number density. A spectral line shape analysis was adopted to extract the Lorentzian component of the emitted line FWHM. This software was applied to different emitted spectral lines (H_α-line, Si I-line at 288.15 nm and O I-line at 777.2 nm) from plasmas formed via interaction of a high peak power laser with a plane solid target in open air.

2. Spectral Line Shape Analysis

2.1. Shape of Emitted Line

The emission spectral line shape is the functional relation between the spectral radiance over the wavelength range. This shape describes the distribution of the light around the central emission wavelength. It could be a Gaussian or Lorentzian, depending on the physical effect considered on the emitting atom or ion [4,5].

The Gaussian line shape can be described by [5];

$$G(\lambda) = A \exp\left(2.7726\left(\frac{\lambda - \lambda_o}{\Delta\lambda_G}\right)^2\right) \qquad (1a)$$

With Gaussian half width in (nm) can be expressed as;

$$\Delta\lambda_G(\text{nm}) = 7.17\times10^{-7}\lambda_o(\text{nm})\sqrt{\frac{T_a(\text{kelvin})}{M_a(\text{amu})}} \qquad (1b)$$

whereas, T_a is the atomic kinetic temperature, M_a is the atomic weight in the units of (amu).

These expressions describe the homogeneous distribution of the spectral intensity around the line central wavelength (λ_o), with amplitude defined by factor A and $\Delta\lambda_G$ is the FWHM. This distribution is best suited to describe Doppler-effect as well as the intrinsic instrumental broadening with $\Delta\lambda_G$ is the measured spectrograph bandwidth.

On the other hand, if the radiance across the line shape is not homogeneous, the distribution of the light around the central wavelength can be best described by the Lorentzian function [5]:

$$L(\lambda) = \frac{0.15915\Delta\lambda_s}{(\lambda - \lambda_o)^2 + (0.5\Delta\lambda_s)^2} \qquad (2)$$

This FWHM $(\Delta\lambda_s)$ is a direct function of the physical processes that can cause such broadening, e.g. Stark effect and/or pressure broadening.

In plasma spectroscopy the actual emission spectral line is often contains a combination of both Gaussian and Lorentzian shapes. This was attributed to the existence of

the different effects of plasma on the measured line shape e.g. Doppler effect, instrumental as well as the Stark effect on the emitting species in the plasma. As a result, the measured line shape should be expressed as the convolution between such effects, which is known as the Voigt line shape [5]:

$$V(\lambda; \Delta\lambda_G, \Delta\lambda_S)$$
$$= \int_{-\infty}^{\infty} G(\lambda'; \Delta\lambda_G)\cdot{}^*L(\lambda - \lambda'; \Delta\lambda_S)\cdot d\lambda' \qquad (3a)$$

This integration is nothing but the convolution function between Gaussian and Lorentzian function, with a FWHM given by:

$$\Delta\lambda_V \approx \frac{\Delta\lambda_s}{2} + \sqrt{\Delta\lambda_G^2 + \left(\frac{\Delta\lambda_s}{2}\right)^2} \qquad (3b)$$

2.2. Measurement of Plasma Electron Density Utilizing Stark Broadening

For the hydrogenic lines appeared in normal LIBS experiments, the Stark effect was found as the dominant mechanism of spectral line broadening [7]. The theoretical calculations of Stark broadening of hydrogenic lines parameters were described in detail in several texts [3-6]. For the linear Stark effect, this broadening manifest itself on form of a Lorentzian line shape having a FWHM $\Delta\lambda(H_\alpha)$, hence, the plasma electron density can be deduced from the spectral broadening of the H_α-line utilizing the following expression [13];

$$n_e(H_\alpha) = 8.02\times10^{12}\left(\frac{\Delta\lambda_s(H_\alpha)}{\alpha_{1/2}}\right)^{3/2}\text{cm}^{-3} \qquad (4)$$

In this expression $\alpha_{1/2}$ is the half width of the reduced Stark profiles in Å, it is a weak function of electron density and temperature through the ion-ion correlation and Debye-shielding correction and the velocity dependence of the impact broadening. Precise values of $\alpha_{1/2}$ for the Balmer series can be found in Ref. [14].

For an elements other than hydrogen and due to collisions with slow electrons and ions, the quadratic Stark effect acts on the half width at half maximum $\Delta\lambda_s$. The electron density can be related to the Lorentzian spectral line half width by [7]:

$$\Delta\lambda_s = \left[1 + 1.75A(1 - 0.75R)\right]\omega_s\frac{N_e}{N_e^{ref}} \qquad (5a)$$

In this equation, $\Delta\lambda_s$ is the electron-impact (half) width, A is the ion broadening parameter, which is a measure of the relative importance of the collisions with ions in the broadening, ω_s is the Stark broadening pa-

rameter. N_e^{ref} is the reference electron density, usually of the order of 10^{16} or 10^{17} cm^{-3}, at which the parameters ω_s and A are calculated [7].

It is worth noting that, the Stark broadening of an isolated non-hydrogenic neutral atom spectral line and ion is mainly due to micro-fields produced by the slow electrons. As a consequence, the contribution of quasi-static ions can be neglected and hence Equation (5a) can be approximated to [7];

$$\Delta\lambda_s = \omega_s \left(N_e / N_e^{ref} \right) \quad (5b)$$

Unfortunately, the situation is not so simple because of the effect of self absorption by non-homogeneous plasma produced by the laser. This is often occur to the emitted spectral lines [15] and might lead to serious errors in the measured density values.

2.3. The Effect of Self Absorption on Line Shape

Self absorption acts to distort the line shape. It increases the line width and decreasing the spectral line intensity [6, 7]. It is originated mostly from the cooler boundary layer which contains most of population of the neutral atoms [6]. For a strong self absorption the line center may exhibits readily recognizable self-reversal [7].

Not very recently, a new method was developed by the author in order to quantify the effect of self absorption to emitted lines in terms of what is known as the coefficient of self absorption (SA) [16]. This coefficient at the line center (λ_o) was originally defined as the ratio of the intensity (counts per sec) of a spectral line subjected to self absorption $I(\lambda_o)$ to that of the same line in the limit of negligible self absorption $I_o(\lambda_o)$ and was expressed as [5];

$$SA = \frac{I(\lambda_o)}{I_o(\lambda_o)} = \frac{1 - e^{-k(\lambda_o)\ell}}{k(\lambda_o)\ell} \quad (6a)$$

However, it was suggested that the same amount (SA) can be expressed on the form of relative spectral line widths of the Lorentzian components of the same line in a two quite different situations of self absorbed line $\Delta\lambda_{s\ell}$ to the case of negligible absorption $\Delta\lambda_{so}$ and therefore, Equation (6a) should reads[16];

$$SA = \left(\frac{\Delta\lambda_{s\ell}}{\Delta\lambda_{so}} \right)^{\frac{-1}{0.56}} \quad (6b)$$

Knowing that the Lorentzian FWHM of any spectral line can be expressed in terms of the electron density $\Delta\lambda \approx 2\omega_s n_e$, then Equation (6b) can further be modified to express the coefficient of the self absorption in terms of the ratio of two electron density values. One is deduced from the distorted line (which of course will yield larger apparent values) $\Delta\lambda_{s\ell} = 2\omega_s n_e (\text{line})$ and the

other is the density of the electrons in the plasma as measured from an optically thin spectral line (The H$_\alpha$-line in our case) $\Delta\lambda_{so} = 2\omega_s n_e (H_\alpha)$. Then Equation (6b) can be modified to:

$$SA = \left(\frac{\Delta\lambda_{s\ell}}{\Delta\lambda_{so}} \right)^{\frac{-1}{0.56}} = \left(\frac{n_e(\text{line})}{n_e(H_\alpha)} \right)^{\frac{-1}{0.56}} \quad (6c)$$

Equation (6c) indicates that the SA coefficient varies from 1 in case of perfectly optically thin line to the limit of zero in case of completely absorbed line [15].

Finally, one has to utilize Equation (6c) in order to calculate the amount of absorption (SA), and then use Equation (6a) to get the corrected value of the spectral line intensity $I_o(\lambda_o)$.

3. Software Program

3.1. Program Orders to Extract Information from the Recorded Line Shape

1) Read the spectrum file data (as exported from camera software);

2) Plot the spectrum in a MatLab7 window;

3) Remove the continuum component under the whole of spectrum;

4) Isolate the line of interest (working line);

5) Calculate the wavelength (λ_{oexp}) at the peak emission;

6) Calculate the spectral shift, from the tabulated wavelength λ_{oTh};

7) Measure the spectral line intensity (Signal height and/or area under curve);

8) Measure the amount of continuum under this line (Background);

9) Calculate the signal to background (continuum) ratio;

10) Building up the necessary functions around this λ_{oexp};

11) Carrying out the necessary convolution between theoretical functions to get the theoretical line shape (Voigt) around this λ_{oexp};

12) Compare the theoretical Voigt function to the isolated measured line shape;

13) Use the necessary equations to calculate the electron density;

14) Repeat the process of comparison until the best fitting is reached, then terminate and give output results;

15) For suspected lines calculate the amount of absorption (SA).

3.2. Program Flowchart

As shown in **Figure 1**, we have started with reading the

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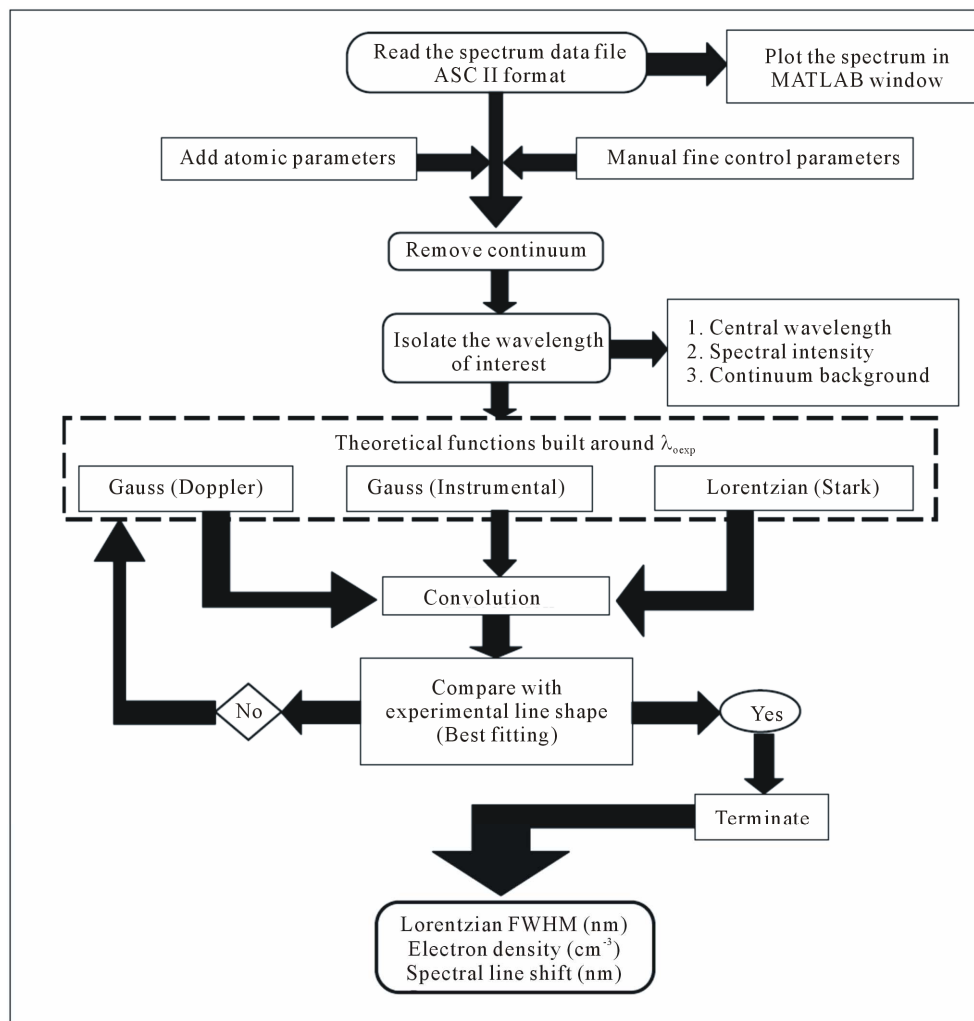in LIBS Experiments via Spectral Line Shape Analysis

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Figure 1. The program flow chart.

exported data from the ICCD camera, and then we feed the atomic data parameters (e.g. wavelength of interest, atomic weight, etc.) and the manual control parameters. Next, we have removed the continuum under the whole the spectrum via creating a new base line. Next we isolate the line of interest, and during this process we calculated the line intensity, and the amount of the continuum appeared under this line and the signal to background ration and also the central line wavelength at the peak of emission. Then, we have built up the required Voigt function via convolution between the Lorentzian and Gauss functions and finally we compare this function to the experimentally measured line shape extracting the Stark component that will be used to measure the electron density at the best fitting. The details of the program can be found at **Table 1**.

4. Results and Discussion

Figure 2 represents the master optical signals in the

range from 200 - 1000 nm as recorded by the ICCD camera program (KestrelSpec® 3.96) and plotted in a MatLab7® window. These spectra were taken at a gate time of 1 μs and arbitrary delay times of 1, 3 and 5 μs.

One can notice the strong continuum component appeared under the whole the spectrum. This continuum is usually attributed to the free-free and free-bound transitions of the quasi free electrons in the plasma and should be removed before processing any optical signal. Also one can notice the decrease in the continuum level as the delay time increases from 1 to 5 μs.

Figure 3 shows the new base line plotted in red color, this line was created via fitting of the whole the spectrum (40001 pixels) to a polynomial function set at the 5th order. One can notice that for every region the cutting level should be manually adjusted. This can be done by the manual control set at program statement number 15. The clean spectrum after subtraction of the continuum is shown in **Figure 4**.
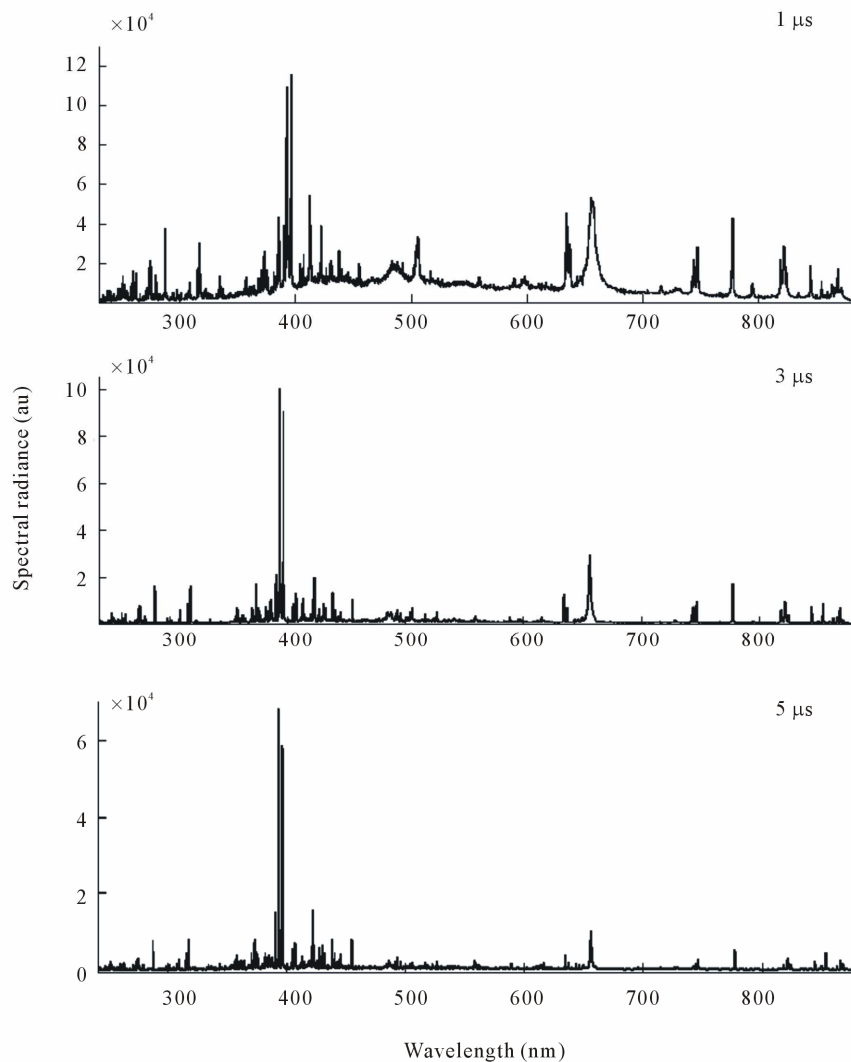
Figure 2. An example of the emitted spectra from plasma at three arbitrary different delay times of 1, 3 and 5 µs.
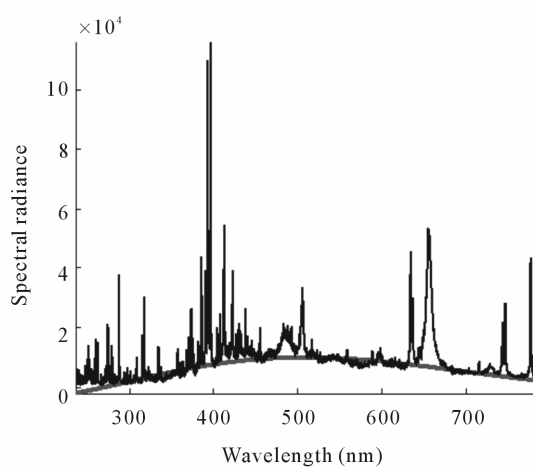

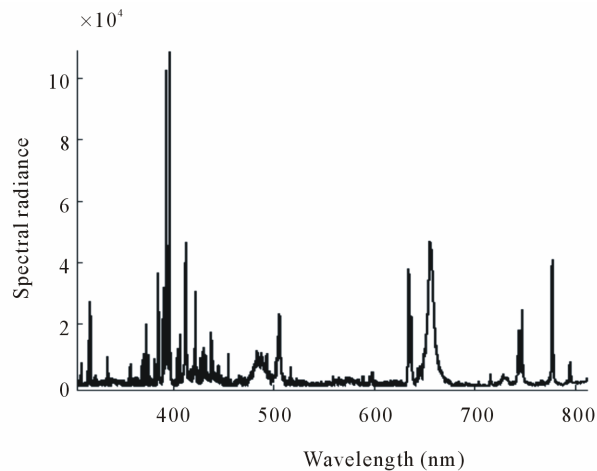**Figure 3. A plot of the master signal (black) and new base line (red).**

Figure 4. A plot of the emission spectrum after subtraction of the continuum component.

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The isolated H_α-line in the master form (data pixel points) is shown at **Figure 5**. The signal analysis will be applied to this optical signal, first we will calculate the spectral radiance and then de-convolute the different contributions to the line FWHM. Peering in mind that the Stark width component will be used to evaluate the electron density, hence, a comparison of this signal to a theoretically Voigt function will be applied.

On the other hand, **Figure 6** shows a plot of the different theoretical functions (Lorentzian and two Gaussian shapes) centered at the experimentally measured central emission wavelength (λ_{oexp}). It is worth noting that the

Gaussian functions can be attributed to the Doppler-effect as well as the instrumental bandwidth of the spectrograph, while the Lorentzian component to the pressure or Stark effect. One can observe that either of the Gaussian components of the line is very small with respect to the Stark component in LIBS experiments, or hence the Doppler component can generally be neglected without too much error. **Figure 7** shows the results of the comparison of the theoretical Voigt line shape (Black curve) to the experimentally measured profile (red curve) at the best fitting.

Figure 8 shows the results of fitting of the Voigt function to the H_α-line profile at two arbitrary delay times of 3, 5 µs, respectively. The repeated application of the program at two different delay times yields $\Delta\lambda_{\text{Stark}} = 1.76$, 1.03 nm, respectively and hence an electron densities of 2.1×10^{17} and 9.5×10^{16} cm^{-3}, respectively.

We have tested the program in order to evaluate the electron density from elements other than hydrogen, e.g. Si I at 288.15 nm and O I at 777.2 nm appeared in the same emission spectra. Noting that, the equation used to evaluate the electron density should be changed, *i.e.* instead of using Equation (4), one should use Equation (5b). The stark broadening parameters of the two lines are taken from tables at Ref. [4], at the given reference electron density. At **Figure 9** we give the results of the application of the program to the Si I and O I at three different delay times namely at 1, 3, 5 µs together with the evaluated electron densities.

Finally, in order to realize the importance of the measurements of the electron densities utilizing different lines arising from plasma produced by laser, one should plot the variation of the electron density as inferred from dif-
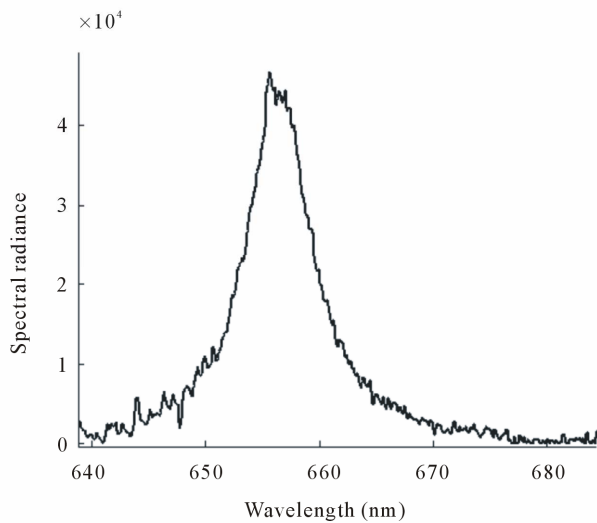

Figure 5. Shown is the isolated master optical emission signal at the H_α-line.
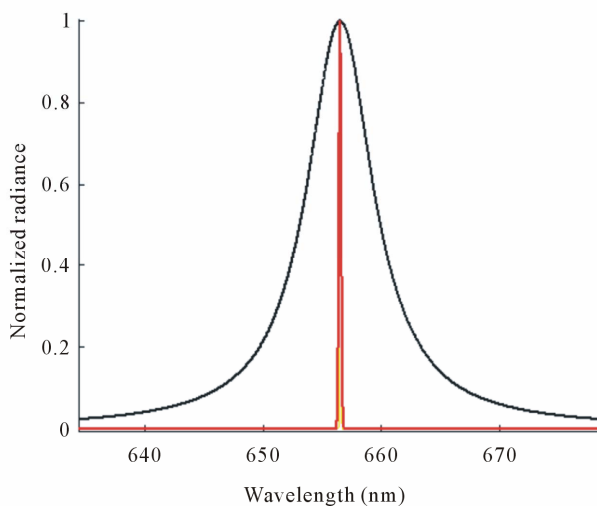

Figure 6. A plot of the Lorentzian function (Drawn in black); the Gaussian function resulted from the instrumental broadening (drawn in red), the other Gaussian resulted from the Doppler-Effect is extremely small.
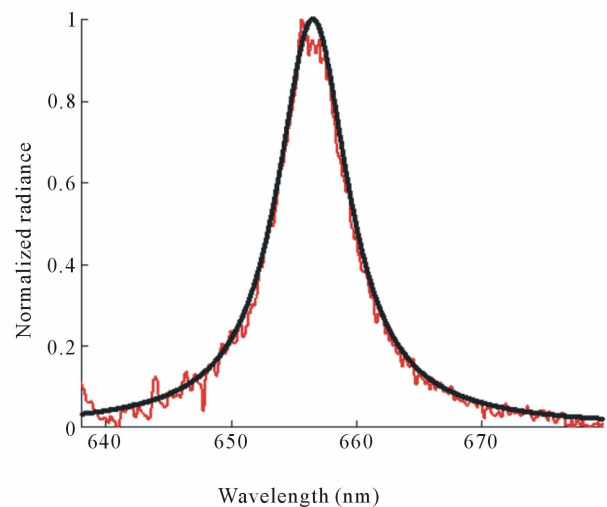

Figure 7. An example of fitting the experimental line profile at the H_α-line (red curve) to the theoretical Voigt function (Black curve).

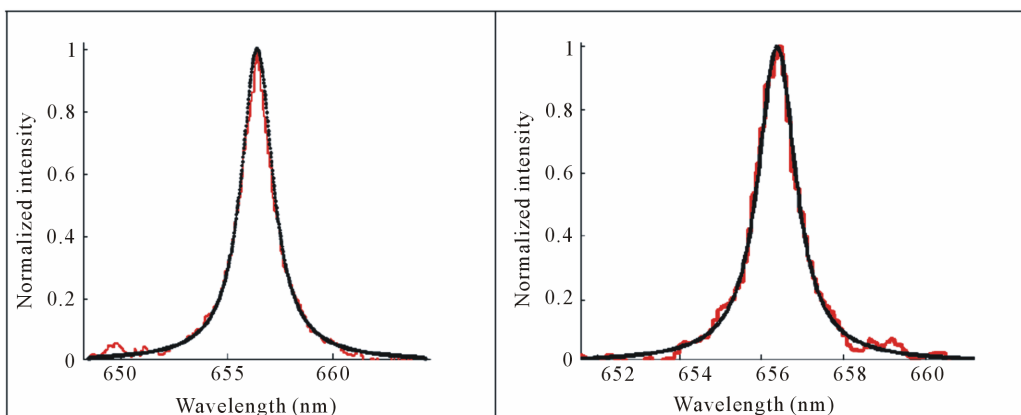**Figure 8. Shown are the results of the fitting of the experimentally measured line profiles of the H$_\alpha$-line to the theoretical Voigt function at an arbitrary delay times of 3, 5 μs (read from left to right) respectively.**
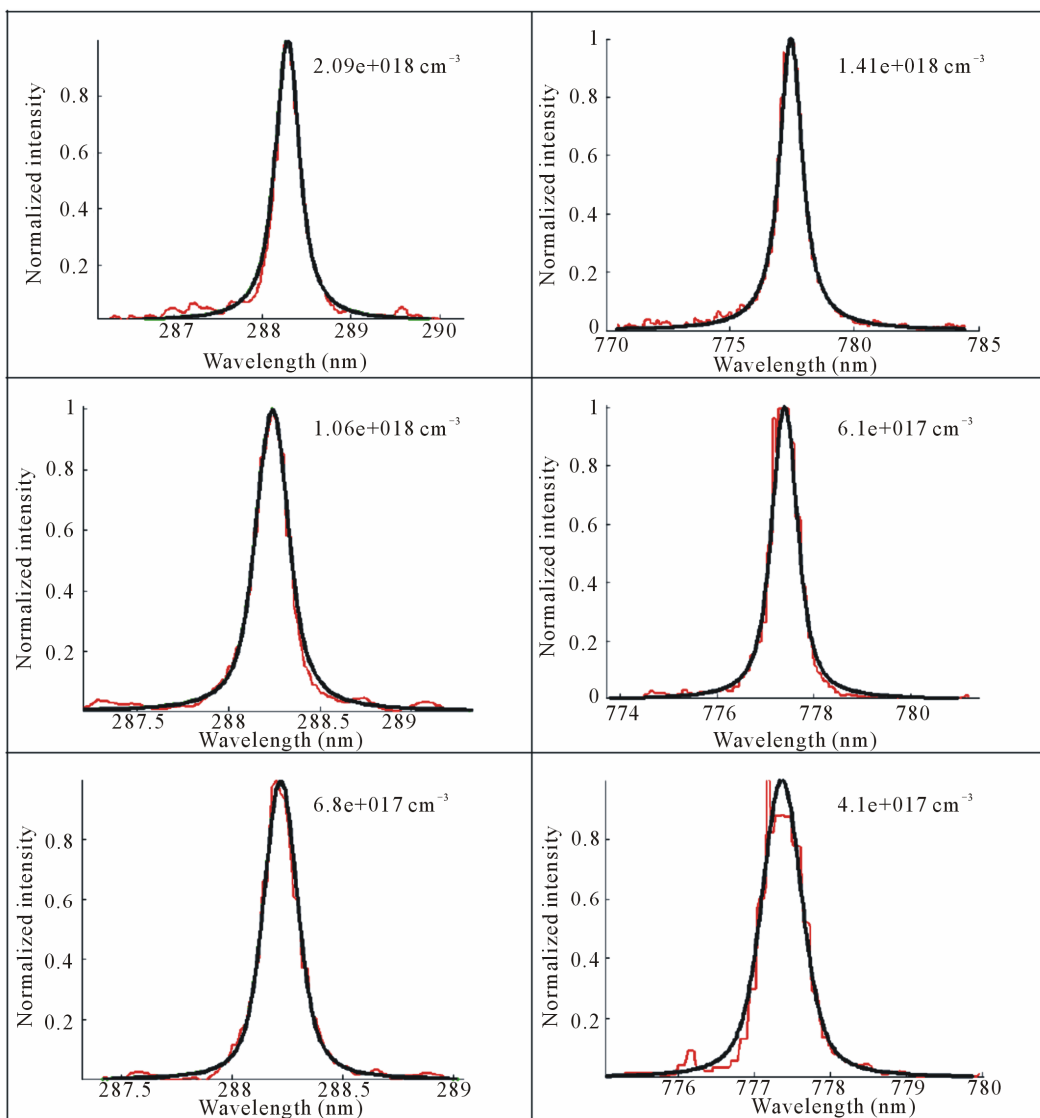

Figure 9. Shown are some examples of the Voigt fitting to the Si I line at 288.15 nm and the O I at 777.2 nm, at three different delay times of 1, 3, 5 μs (read from top to bottom).

ferent lines. **Figure 10** represents the results of the estimated electron density with delay time. From the figure one can conclude that the line at Si I suffering from optical thickness while this is not the case of the O I at 777.2 nm. This is because one can notice the strong deviation of the electron density calculated from the Si I-line at 288.14 nm and the moderate deviation of the O I-line at 777.2 nm from the density as calculated from the H_α-line. This indicates that both lines are subjected to some self absorption.

With the help of expression (6c), after comparison of the calculate electron density from one line to the same amount as evaluated utilizing the H_α-line one can calculate the amount of optical thickness of the plasma at each line and correct the intensities of either line which lies after the scope of this article.

5. Conclusion

We have developed simple routine software used to evaluate the electron density utilizing the spectral line shape analysis to the light emitted from plasma. This routine is based on comparison of the measured line shape to a theoretically built Voigt function. This enables us to extract the stark component contribution to the line width, hence the calculation of the plasma electron density. The electron density was evaluated utilizing different spectral lines emitted from the plasma under the same condition e.g. the H_α-line (that was used as a reference line in the measurement of the electron density) as well as Si I-line at 288.15 nm and the O I-line at the 777.2 nm.
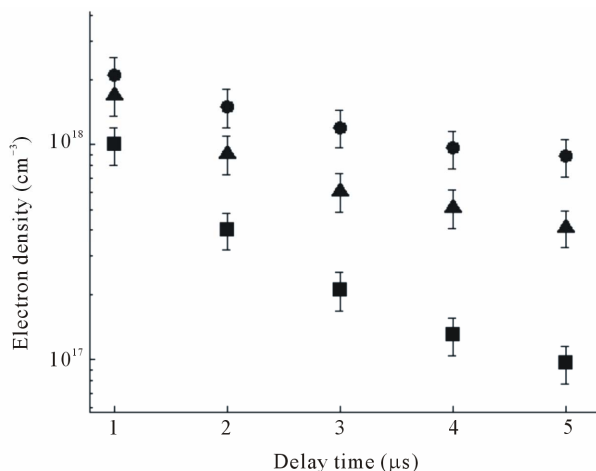

Figure 10. A demonstration to the temporal variation of the finally calculated electron density utilizing the program with delay time, squares represent the calculated electron density from the H_α-line, triangles are the same density as measured from the O I line at 777.2 nm and the solid disks are the electron densities as calculated from the Si I-line at 288.15 nm.

The higher densities showed by lines other than hydrogen was attributed to the presence of optical depth of the plasma to these lines.

6. Notations

1) In order to change the wavelength of interest (*i.e.* to apply the analysis to another line) one has to assign the new wavelength of interest at line number 4.

2) For lines other than the H_α-line, one has to use Equation 5(b) instead of Equation (4) and use line number 33 instead of line number 32 (pause line 32 by using the % sign at the start of the line) together with assignment of the reference electron density (N_r) and Stark broadening parameter (ω_s) at lines 11,12.

3) From our experience to handle the LIBS spectra under our condition of the laser energy and duration the expected temperature is almost around 1 eV and hence the Doppler FWHM is almost centered on 0.04 nm that can be neglected.

4) One more option that can enhance precision of the fitting is to change the value of the controllable precision parameter at line 16.

5) In order to examine somewhat line against the effect of absorption, one has to run the program two times in series. The first run to calculate the density utilizing the H_α-line, and the next to run the program to calculate the same density using the suspected line. Then the application of Equation (6c) will evaluate directly the amount of self absorption. If the SA value is found in the range (0.8 - 1) the line is considered as optically thin [15], lower values of *SA* means that the lines is thick and need to be corrected.

6) The correction of spectral intensity against the effect of self absorption can be carried using Equation (6a) in order to evaluate $I_o(\lambda_o)$.

7) Lines (13 - 16) completely enables one to control the fitting to the experimental line shape.

7. Acknowledgements

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Appendix A

Program statements in MatLab7®.

Table 1. Description to order at each line.

Line No.	Order
01	close all, clear all
02	load filename.txt
03	L = filename (:, 1); I = filename (:, 2);
04	Waveleng_of_Int = 656.27; % in nm units
05	Expected_Temp = 1; % in eV units
06	Mol_Mass = 1; % Molecular mass in amu units
07	DLG1 = 0.12; % Instrumental Bandwidth in nm units
08	Ne_Step = 1e16; % in e/cm3 units
09	Expected_Density_Range = [1e16:Ne_Step:5e18]; % in e/cm^3 units
10	fit _order = 5; % polynomial fitting order
11	Nr = 1e17; % Reference density in e/cm^3 units
12	Ws = 0.0044; % Stark broadening parameter in nm units
13	Range = 1000; % Number of pixels to cover the line
14	Jitter _Shift = –35;
15	Cutting _Level = –3000;
16	Precision = 0.0000024;
17	p = polyfit (L, I, fit _order)
18	pp = Cutting_Level + polyval (p, L);
19	ppp = abs(I-pp);
	%%%
20	x1 = find (L == Waveleng_of_Int-1); x2 = find (L == Waveleng_of_Int + 1);
21	L1 = L(x1: x2);
22	[y1 y2] = max (ppp(x1: x2));
23	Lo = L1 (y2-Jitter_Shift);
24	[Y1 Y2] = max (pp(x1: x2));
25	SBg = y1/(Y1);
26	k = find(L == Lo);
27	WL = L(k − Range : k + Range);

Continued

```
28        Hi = ppp(k − Range :k + Range);

29        Bg = pp(k − Range :k + Range);

30        % plot (WL, Hi./max(Hi), "go"), hold on

31        for Ne = Expected_Density_Range;

32        DLL = ((Ne./31.622.*2.84e15).^0.66666); % Ha-Line

33        % DLL = (Ws.*Ne)./Nr; % Lines other than hydrogen

34        Lor = (0.15915.*DLL)./(((DLL. /2). ^2)+((WL-Lo).^2));

35        35. % plot (WL, Lor./max (Lor), "b"), hold on

36        G1 = 0.93943.*DLG1.*(exp(−0.5*((WL-Lo)./DLG1).^2));

37        % plot (WL, G1./max(G1), "y")

38        DLG2 = 7.17e − 7.*Lo.*sqrt(((11600.*Expected_Temp)./Mol_Mass));

39        G2 = 0.93943.*DLG2.*(exp(−0.5.*((WL-Lo)./DLG2).^2));

40        % plot(WL,G2./max(G2), "r")

41        V1 = conv(G1,G2);

42        [yo1 yo2] = (max(V1));

43        V2 = V1(yo2 − Range :yo2 + Range);

44        % plot(WL,V2./max(V2), "r")

45        Vo = conv (V2, Lor);

46        [yoo1 yoo2] = (max (Vo));

47        Vo2 = Vo (yoo2 − Range: yoo2 + Range);

48        Rss = sqrt(sum(((Hi./max(Hi)-(Vo2./max(Vo2)).^2));

49        if Rss < Precision

50        Spectral_shift = Lo-Waveleng_of_Int;

51        [h hh] = size(WL); Area = sum(Hi(1:h-1).*diff(WL));

52        Electron density = ne

53        Lorentzian_FWHM = DLL

54        Sgnal_Height = y1

55        Signal_To_Background = SBg

56        Intensity = Area

57        figure(110), plot(WL,Hi./max(Hi),'r-,WL,(Vo2)./(max(Vo2)),'g.')

58        xlabel ('Wavelength(nm)'), ylabel (' Normalized intensity (au)')

59        break,

60        end, end
```

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Appendix B

Program Statement Function

Line No	Task Description
1	Close and clear any programs running at the Matlab working space
2	Load the data file (ASC II format)
3	Assign the wavelengths from 200 nm to 1000 nm with a step difference (resolution) of 0.02 nm per pixel, to single column matrix which is now contains 40,001 pixels, call it matrix-L. Also, assign the signal height at each wavelength to single column matrix which also contains 40001 pixels, call it matrix-I
	Manual Control Parameters
4	Specify the working wavelength in nm units
5	State the expected electron temperature
6	State the molecular mass of atom or ion of the element that emits light in amu units
7	Assign the instrumental bandwidth as measured in units of nm
8	Assign the step in electron density range (PRECISION IN MEASURMENTS)
9	Assign the expected lower and higher density values with step as stated at line 8
10	Assign the order of the used polynomial function for fitting to the whole spectrum in order to create the new base line
11	For elements other than hydrogen, assign the reference electron density value
12	For elements other than hydrogen, state the Stark broadening parameters as taken from standard tables
	Fitting Control Parameters
13	Assign the number of pixels that can cover the line to wings
14	Assign the number of pixels used to correct the peak wavelength against pulse jitter
15	State the amount of the manual cutting level (this may be changes from one line to the other in the same working spectrum)
16	State the precision needed for the fitting of spectral line to the Voigt function
	Creation of New Base Line
17	Use the built-in polynomial function, fit the whole the spectrum to an order defined before at line number 10
18	At the best fit to the emission spectrum, evaluate the polynomial coefficients, this new pp function will act as the NEW BASE LINE. This new base line can be further detuned via addition or subtraction of a certain constant as mentioned before at the (Cutting Level) specified at line number 15. Upon detuning to this factor one can reach the best cutting level at the line wings, call the resulted new base function as matrix-pp. This matrix function is actually the continuum emission component, which is resulted mainly from the free-free and free-bound transition and should be subtracted before application of analysis to the line shape.
19	Subtract this new base (matrix-pp) from the master spectrum (matrix-I) to get a clean spectrum (matrix-ppp) without the unnecessary continuum component appeared under the line of interest.
	Isolation of the Spectral Line of Interest
20	Utilizing the wavelength matrix (L), choose the pixel point "x1" that lie before the wanted line of interest and choose the pixel point "x2" lie after the line of interest
21	Create a single matrix of new wavelengths "starting from pixel number x1 and ended at pixel number x2" call this new wavelength region as matrix-L1
22	In the same range from pixels (x1: x2) find the maximum height (y1) from the matrix (ppp) without continuum, this is the line intensity in units of counts/sec and the corresponding pixel number y2 of the peak height
23	Calculate the wavelength corresponding to the pixel number y2 and call this wavelength as Lo (λ_{oexp}) taking into account any jitter in the peak wavelength
24	In the same range from pixels (x1: x2) find the maximum height from the matrix (pp) which represent the continuum intensity (Y1) in units of counts/sec

Continued

25	Calculate the signal to background (y1/Y1)
	Built up the Necessary Theoretical Functions around λ_{oexp}
26	From the wavelength matrix L, find the pixel number (k) corresponding to λ_{oexp}
27	Create a new wavelength region centered around λ_{oexp} and extended by number of pixels specified previously by (Range—at line number 13)
28	Utilizing matrix (ppp) of signal heights and free from continuum, find the new heights in the same range corresponding to the new wavelength WL regime *i.e.* in the same region defined by statement range at line 13
29	Utilizing matrix (pp) of background continuum, fine the new heights in the same range corresponding to the new wavelength WL regime *i.e.* in the same region defined by statement range at line 13
30	Plot, if necessary, the experimental isolated line in the new range defined by new wavelength regime WL and the corresponding signal heights Hi
	The Theoretical Functions 1. Lorentzian Function
31	With the help of the properties of the "FOR-loop" let the electron density Ne is the free running parameter according to values previously defined at line number 9, together with the precision step at line 8
32	For the hydrogen H_α-line only use equation 4 at the text to calculate the Lorentzian FWHM in nm
33	For lines other than the hydrogen H_α-line, use this equation 5b to calculate the Lorentzian FWHM in nm
34	Calculate the Lorentzian function according to line FWHM defined in the previous step
35	Plot, if necessary the theoretical Lorentzian function centered around λ_{oexp} in the new range defined by wavelengths WL and signal heights Hi
	2. Gauss Function Resulted from the Instrumental Bandwidth
36	Calculate the Gauss function according to line FWHM defined line number 7
37	Plot, if necessary the theoretical Gauss function centered around λ_{oexp} in the new range defined by wavelengths WL and signal heights Hi
	3. Gauss Function Resulted from the Doppler Effect
38	Calculate the line FWHM according to Doppler effect centered around λ_{oexp} in the new range defined by wavelengths WL and signal heights Hi at the expected electron temperature specified at line number 5
39	Calculate the Gauss function according to line FWHM defined in the previous step
40	Plot, if necessary the theoretical Gauss function centered around λ_{oexp} in the new range defined by wavelengths WL and signal heights Hi
	4. Start Convolution between the Different Functions
41	Start with convolution between the two Gauss functions G1, G2
42	Calculate the pixel number corresponding to the maximum of the new function V1 and call this number as yo2
43	From this function V1 extract the required number of pixels just to cover the spectral line according to Range specified to line 13, call this function as V2
44	Plot, if necessary the theoretical V2 function centered around λ_{oexp} in the new range defined by wavelengths WL and signal heights Hi
	5. Carry a Convolution between V2 and the Lorentzian Function
45	Convolute the two functions V2 and Lorentzian function (Lor), call new function as Vo
46	Calculate the pixel number corresponding to the maximum of the new function V1 and call this number as yoo2
47	From this function Vo extract the required number of pixels just to cover the spectral line according to Range specified to line 13, call this function as Vo2
48	Compare between the theoretically built normalized Voigt function (Vo20 and the experimentally normalized measured line profile Hi according to the principle of least square fitting method. Call the residual number as RSS
	6. Utilizing the Conditional (IF-Statement)
49	If, the residual number at line 48 corresponding to the fitting, is lower than a certain level defined by order precision at line 16

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50	Calculate the spectral shift
51	Evaluate the area under the experimentally measured profile
52	Evaluate the electron density at the best fit
53	Evaluate the Lorentzian FWHM in nm at the best fit
54	Evaluate the signal height at the best fit
55	Evaluate the background at the best fit
56	Evaluate the spectral intensity as area under curve at the best fit
56	Plot the final results of comparison between the theoretical function and the experimentally measured line profile
58	Break the loop
59	End the first loop started at line 49
60	End second loop started at line 31