

C\textsubscript{2} Swan spectrum used as a molecular pyrometer in transferred arc and the influence noise to signal ratio on the temperature values.

H NASSAR
Lebanese University, FSP, section IV, Karak Zahlé, Lebanon.
nassar_hossein@hotmail.com

Abstract. The C\textsubscript{2} Swan system molecular emission spectrum is frequently observed in arc plasmas containing hydrocarbons. The spectra emitted from 5 kw in the transferred arc reactor at atmospheric pressure by CH\textsubscript{4}/CO\textsubscript{2}/Ar mixture are recorded with the help of an optical system consisting of a linear CCD array coupled with 2m spectrometer. The rotational temperature of 4300±300K is found from the experimental Abel inverted spectra in the arc center after a point–to–point comparison of the spectrum with a computer simulated one. The influence of the noise to signal ratio has been studied, if the noise to signal ratio is about 10% we found an error of 7% at temperature 3000K and 10% at 6000K.

1. Introduction
The Swan band of C\textsubscript{2} molecule is a good tool for diagnosing plasmas containing this molecule, the molecular constants and the lines structure are well-known, and it is present in most of the plasma sources containing hydrocarbon for a temperature between 3000K and 6000K. Pellerin in 1997 use Swan band spectrum for temperature measurements and to answer some questions on thermodynamic equilibria in a plasma produced from the CH\textsubscript{4} +CO\textsubscript{2} mixture in a transferred arc[1]. Bontemps-Faure in 1997, uses this system to study thermodynamic state in thermal plasmas[2]. In (1998) Laffon [3] use the C\textsubscript{2} (1, 1) and (0, 0) bands to measure the temperature in Comet Hyakutake C/1996 B2. It is shown that the temperature increases with cometo-centric distance. Babou, in 2008, have determined the profile of temperature in CO\textsubscript{2} and CO\textsubscript{2}/N\textsubscript{2} plasmas produced by a microwave torch at atmospheric pressure using this band [4].

In the previous publications, we have proposed a numerical method based on the simulation of molecular spectrum for studying the distribution temperature in modified arc Maeker[5] and[6], and in transferred arc[7]. To determine N\textsuperscript{+2}/N\textsubscript{2} ratio and the temperature distribution in Glidar[8], we have made the simulation of both systems first negative and second positive one simultaneously.

In this paper, we have used this method based on the simulation of the (0,0) band of C\textsubscript{2} molecular Swan system. The method proposed permit to evaluate, by comparing point to point a real spectrum with the simulated one, temperature and apparatus function, approximated by the gauss function (the half-width at 1/e height). The real spectrum is emitting from plasma produced in a transferred arc in CH\textsubscript{4}+CO\textsubscript{2} mixture. Moreover, it is shown, by noised spectra simulation, the influence of noise to signal ratio at the calculated temperature values.
2. Simulation of the $d^3\Pi_g - a^3\Pi_u$ spectrum of $C_2$

2.1. The Swan system of $C_2$ molecule

A complete description of the spectral terms of the diatomic molecules may be found, e.g. in [9] and [10], or in our previous publications [6] and [8]. The Swan system of homo-nuclear molecule $C_2$ corresponds to radiative transitions between the $d^3\Pi_g$ and $a^3\Pi_u$ electronic state ($\Lambda = 1$) at 2.59 ev and 0.19 ev respectively. We are interested in the visible (5138Å, 5170Å) spectral range covering the (0,0) band. The coupling is type ‘(a) Hund case for lower $J$ values and type ‘(b) hund case’ for $J$-values higher than 15 [10].

The absolute rotational emission line intensity of the molecule is given by

$$
\varepsilon_{nl} = C\sigma^4 S_{j,j'}, \exp \left( -\frac{h c F(J')}{KT} \right)
$$

Where $C$ is a normalization constant, $\sigma$ is the wave number, $S_{j,j'}$ is the Hönl-London factors, $h$ and $c$ are the conventional physical constants, $F(J)$ is the spectral terms and $T$ is the temperature. (marks concern the lower spectral term and the marks ' are for the upper one). Formulae for $S_{j,j'}$ factors for the intermediate a-b Hund case are taken from Kovacs [10] and the spectral terms are those of Budo [11].

2.3. Numerical simulation of band (0,0)

Line intensities are calculated when a state of thermodynamic equilibrium is fully reached and the corresponding temperature of the gas, considered from a macroscopic and thermodynamic point of view, are the same. In reality, within laboratory plasmas, we usually have to deal with a local thermal equilibrium state instead of thermodynamic equilibrium state.

It is possible, when the population of discrete energy levels follow Boltzmann's Law, to attribute a corresponding temperature for each corresponding energy distribution; electronic, $T_e$, vibrational $T_v$ and rotational $T_R$. In a non-equilibrium plasma $T_p$, $T_v$ and $T_R$ may differ from the kinetic temperature $T_g$ of heavy species. Taking into account the strong coupling between translational and rotational energy states, the temperature derived from experiments is, in a general case, close to the gas kinetic temperature [12] and [13]. Thus, $T_g$ can be deduced from $T_R$, measured by using the rotational structure of molecular spectra.

All the spectral constants are taken from Herzberg [9]. Computed spectrum of individual lines for a given temperature is then convoluted with our apparatus function approximated by the gauss function whose $DX$ (the half-width at 1/e height):

$$
I_0 = \int_{\nu_0-DX}^{\nu_0+DX} I_{\nu_0} \exp \left( -\frac{(\nu - \nu_0)^2}{DX^2} \right) d\nu
$$

Where $\tau = 2.5$ DX and $\nu_0$ is the wave number of the line.

An integrated cell (pixel) of simulated spectrum is chosen according to the cell of experimental spectrum under consideration. We can, following the situation, group several cells in one.

Practically, for each given set of values (DX, $T_R$), the line intensities of this band are normalized to its maximum. Examples of simulated spectra, normalized to 100, are shown in figures 1 and 2 for different sets of (DX, $T_R$) values.

A quick analysis of these simulated spectra shows that the apparatus function has essentially influenced the resolution of the rotational line structure. Particularly, if DX is too high, only the shape of the band...
can be used to determine the rotational temperature. The rotational temperature has a significant influence on the rotational line structure.

3. Numerical method for rotational temperature evaluation
To evaluate the $T_r$ from a given real spectrum, we have chosen to compare this spectrum point-by-point with spectra simulated at different values of $DX$. In our experiments the following procedure was applied. (i) The measured spectrum was corrected for the continuous background, which was assumed to be linear in the studied spectral range. (ii) The experimental spectral intensity was normalized to the maximum value, which was set to 100. (iii) The experimental data were compared with that of the simulated spectrum. The minimization procedure was used to minimize $E(T_r, DX)$ as a function of $T_r$ and $DX$ defined as:

$$E(T_r, DX) = \frac{1}{N} \left[ \sum_{i=1}^{N} \left( I_i^* - I_i \right)^2 \right]^{1/2}$$  (3)

$I_i^*$ and $I_i$ are respectively the intensities of the real and simulated i-th pixel of the spectrum containing N points. If the choice of the spectrum reference origin (background) is a bad one, the result will be affected. To avoid this error, we fix several origins, and our computer program searches the best origin to find the $E(T)$ at minimum.

4. Application to simulated noisy spectra
In order to test the sensitivity of the temperature estimator, we applied this method when a noisy spectrum was used instead of the experimental one. The synthetic spectra were calculated for known apparatus functions, temperatures, and noise was introduced using a random number generator. Examples of simulated spectra noised, normalized to 100, are shown in figure 3 for different sets of N/S ratio. We can see that the rotational spectra are very deformed for the high N/S values.
Calculations were performed for noise-to-signal ratios N/S equal to 1%, 5%, 10% and 20% and for temperatures of 3000 and 6000 K. The results obtained are given in table 1.

| Noise/signal % | 3000k | 6000k |
|----------------|-------|-------|
| 1%             | 1.5%  | 3%    |
| 5%             | 4%    | 7%    |
| 10%            | 7.0%  | 10.0% |
| 20%            | 11.5% | 18.5% |

The results are satisfactory since the relative error in the temperatures is of the same order of magnitude as the noise-to-signal ratio, even if the last one was relatively high.

5. Experimental set-up

5.1 Reactor
The reactor consists of an arc chamber to which an Argon plasma jet of 4 mm diameter emerges through a 2 kw plasma torch nozzle considered as a first anode. This jet makes a first ionization stage. Another tubular transfer anode (5 mm of internal diameter) put at 20 mm from the nozzle aperture allows to obtain a DC transferred arc in which methane and carbon dioxide gases are introduced (see figure 4). Both copper anodes as well as the torch tungsten cathode are water cooled. The transferred arc chamber is fed at atmospheric pressure by CH₄/CO₂ = 1 (molar ratio) gas mixture at 10 sml flow rate. The electrical power supplied to the arc is 5 kw.

5.2 Spectral recording system
The C₂ emission spectra are observed with the help of a 2-meter monochromator equipped with a 1200 grooves/mm grating couples with an optical analyzer based on Thomson linear CCD array (1728 pixels of 13.39 m). The transferred arc column at the half of its lengths is scanned through a quartz window by a step-motor desk computer moved optical system at 12 points at 0.45 mm step following Y axis (figure 5).
6. Results
Twelve spectra records (655 wave lengths points each) were Abel inverted in order to present a local intensity distribution as a function of the radial distance from arc column center. Such distributions are then compared to spectra simulated at large temperature ranges. Three examples of real (experimental) spectra and corresponding simulated one are shown in figure 6, figure 7 and figure 8. The resulting rotational temperature profile in the transferred arc column is shown on figure 9.

Figure 6. Example of an experimental spectrum in the centre of the arc (after the Abel inversion), and corresponding simulated spectrum.

Figure 7. Example of an experimental spectrum at 0.9 mm from the arc column center (after the Abel inversion), and corresponding simulated spectrum.

Figure 8. Example of an experimental spectrum at 1.8 mm from the arc column center (after the Abel inversion), and corresponding simulated spectrum.

7. Discussion and conclusion
The rotational temperature of about 4900 ±300 K has been found from the experimental spectrum in the arc column center while at the column fringes the temperature drops to 3200±350 K at 1.8 mm from the axis. This last point was obtained from a quite weak and nosily spectrum (N/S=20%). Looking at different spectra in real points, we observe that the emission is maximum (the signal is very strongest N/S<1%) at 0.9 mm distance from the arc center where the temperature is around 4200 K which means...
that the concentration of carbon molecule is maximal in this point. The concentration of carbon molecule decreases slightly, approaching the center of the arc where the temperature is about 4900K and N/S = 5\%. Instead, this concentration is greatly reduced in periphery zone of the arc, where the temperature is around 3200K and N/S > 20\%.

Figure 9. Radial distribution of the rotational temperature in transferred electric arc column in Ar/CO2/CH4 Mixture.

A calculation based on Limoges's computer program [14] of the complete thermodynamic equilibrium for the same CH4/CO2/Ar gas mixture (H/C/O/Ar = 1/0.485/0.463/0.168 in moles) shows that the C2 molecule concentration in plasma reaches its maximum at about 4200 K and then drops by two orders of magnitude at about 3200 K. The temperatures for which this molecule can be used as a “thermometer” cover therefore a region from about 3000 to 5000 K.

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