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Self-consistent modeling for estimation of the reduced electric field in a DC excited diffusion controlled CW CO_2 laser

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ABSTRACT

The results of a numerical simulation method that estimate various discharge parameters in the positive column of a DC glow discharge controlled by ambipolar diffusion are presented. The parameters like reduced electric field (*E/N*), electron temperature, ionization rates, ambipolar diffusion losses and the average gas temperature were numerically evaluated for several mixtures of CO_2, N_2 and He in low pressure regime. The estimated *E/N* value which is a primary governing parameter of positive column was verified experimentally using a double probe in diffusion controlled CW CO_2 laser for a variety of CO_2, N_2 and He mixtures. The role of auxiliary ionization source like pulser used for pre-ionization and its effect on the steady state *E/N* value was also studied. A reasonably good agreement was found between the theoretical and the experimental results. Based on the results of this simulation a zigzag folded, diffusion-cooled, 500 W CW CO_2 laser has been designed and developed for research in gas phase nanoparticle synthesis.

1. Introduction

With the evolution of compact, high power fiber and solid state lasers coupled with the advantage of fiber delivery, these lasers are often preferred over CO_2 lasers for various industrial applications. However, in applications specific to CO_2 laser wavelength i.e. 10.6 μm, there is no choice. One such current application where the wavelength of CO_2 laser is important is gas phase synthesis of nanoparticles [1–3]. The CO_2 laser is absorbed in gaseous precursors or sensitizers because of its strong overlap with the absorption bands of the molecules. Absorption of laser leads to heating of the interaction zone resulting in gas phase pyrolysis and the subsequent formation of various nanoparticles. The laser power typically used for laser pyrolysis ranges from 0.1–1 kW. Higher power CO_2 laser however, give higher yield of nanoparticles often required for large scale production of nanoparticles. One such application is solar water splitting for hydrogen generation using the concept of artificial leaf [4]. The artificial leaf is mainly an electrode coated with semiconductor material in the form of nanoparticles which generates electron hole pair on irradiation of light on it. Such electrodes in contact with water could split it resulting in formation of hydrogen. The potential semiconductor material for this key application is TiO_2.

A setup for laser based gas phase pyrolysis reactor for generation of TiO_2 nanoparticles has been developed. For this purpose an indigenous CO_2 laser of power more than 500 W was required. To fulfill this objective a diffusion-cooled, long active medium length CW CO_2 laser with planar zigzag resonator has been developed [5]. The advantage of such a system is that it is simple in design as no gas blower and heat exchangers are required for its operation. However, the alignment of the optical resonator is somewhat sensitive due to its long length. The resonator was made less sensitive to alignment by using planar zigzag resonator with curved folding mirrors [5]. In order to extract maximum power from such laser system it was required to optimize the gas mixture ratio and output coupler reflectivity. The optimum gas mixture ratio is one which gives maximum small signal gain g_o. Once the gain and saturation intensity are known, the optimum output coupler reflectivity can be found using Rigrod's formula [6].

For a given gas mixture, the gain can be estimated by solving the rate equations, but requires the knowledge of excitation rates which in turn depend on the reduced electric field i.e. *E/N* (*E*=Electric field, *N*=Neutral species number density) in the positive column. The reduced electric field controls the Electron Energy Distribution Function (EEDF) and hence the average

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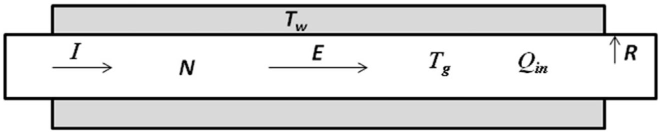

Fig. 1. Water cooled cylindrical discharge tube. R: Radius of the tube, T_w: Water temperature, T_g: Average gas temperature, N: Neutral species number density, Q_{in}: Input power density, I: Discharge current, E: Electric field in the positive column.

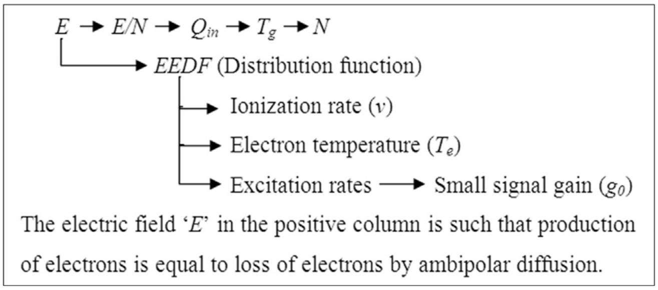

Fig. 2. Flow chart indicating the role of electric field E in the modeling of diffusion controlled laser system.

electron energy [7–9]. In the glow discharge, established in the cylindrical diffusion controlled CW CO_2 laser discharge tube, the steady state E/N value in the positive column is governed by the balance between the ionization and ambipolar diffusion loss rate of electrons [10]. Modeling of diffusion controlled CW CO_2 lasers thus relies on the value of electric field E that exists in the positive column of the glow discharge established in a laser gas mixture. The various parameters of importance for modeling of such glow discharge pumped laser systems are depicted in Fig. 1.

The flow chart to illustrate the role of E in the positive column of CW CO_2 laser is shown in Fig. 2. It is clear from Fig. 2 that, the starting point in the modeling of diffusion controlled CW CO_2 laser is the electric field E in the positive column which is a function of gas mixture ratio, gas pressure, gas temperature, tube diameter and discharge current.

In the absence of the knowledge of main discharge controlling parameter E or E/N, one relies on the published value of the E/N in the positive column of commonly used gas mixtures such as CO_2:N_2:He::1:1:8 [7]. However, the optimum gas mixture for a given diffusion controlled CW CO_2 laser may differ from 1:1:8 gas mixture [11–13]. In such cases, modeling and analysis of such systems demand the knowledge of electric field E in the positive column so that other parameters required for complete modeling can be evaluated as shown in the flow chart given in Fig. 2. The simplest approach is to use the Langmuir double probe and find experimentally the electric field in the positive column [14,15]. However, this makes the theoretical modeling less flexible as it demands experimental input to start with. On the other hand if the electric field in the positive column could be derived theoretically from the first principle, the power of modeling such laser systems increases manifold. It can be shown theoretically that such E/N value is established in the positive column which satisfies the equation given below [10,16];

$$\frac{\nu}{\mu^+} = \frac{K\,T_e}{e}\left(\frac{2.405}{R}\right)^2 \tag{1}$$

where, ν=ionization rate (1/s); μ^+=mobility of positive ion (cm^2/V s); K=Boltzmann constant (J/°K); T_e=average electron temperature (°K); e=electronic charge (C); R=discharge tube radius (cm).

The ionization rate (ν) can be found easily if the EEDF is known as a function of E/N for a given gas mixture. The diffusion loss rate of electrons is governed by ambipolar diffusion coefficient D_a which is expressed as [17];

$$D_a = \mu^+\frac{K\,T_e}{e} \tag{2}$$

Estimation of D_a thus requires μ^+ and T_e as a function of E/N. Electron temperature T_e can be calculated using EEDF but value of μ^+ has to be taken from the reported values in the literature [18,19]. When Eq. (1) is applied to CO_2 laser gas mixtures then it takes the following form [15,16];

$$\frac{\nu_C}{\mu_C} + \frac{\nu_N}{\mu_N} + \frac{\nu_H}{\mu_H} = \frac{K\,T_e}{e}\left(\frac{2.405}{R}\right)^2 \tag{3}$$

where, ν_C, ν_N, ν_H are ionization rates of CO_2, N_2 and He gases respectively by electrons in the discharge. These ionization rates are calculated with the help of EEDF [20]. The μ_C, μ_N, μ_H are mobilities of CO_2^+, N_2^+ and He^+ ions respectively in the laser gas mixture [18,19]. In the published literature, experimental values of E/N in the positive column of CW CO_2 laser discharge can be found [21–23]. Theoretical estimation of electric field in diffusion cooled CW CO_2 laser using Boltzmann transport equation and ambipolar diffusion loss of electrons together with recombination of negative ions has been reported by Galeev et al. [24]. A good matching between the theoretical and experimental results has been reported by Galeev. However, the reason for assuming the presence of negative ions and their concentration higher than that of electrons is not very clear. A similar approach to estimate the electric field in the positive column of glow discharge in flowing hydrogen has been also reported by Brunet et al. [25].

In this paper, theoretically calculated E/N values in the positive column of typical gas mixtures in diffusion controlled CW CO_2 lasers are presented along with its experimental verifications. A slightly different approach has been adopted here than the one reported by Galeev [24] and attempts have been made to identify and incorporate the parameters which could improve the matching between theoretical and experimental results. The experimental values of E/N were obtained using Langmuir double probes placed in the positive column. To show the validity of the model adopted by us, electric field in the positive column was measured and theoretically estimated for variety of gas mixtures under different operating conditions. The simulated results were used to design a diffusion cooled zig-zag folded 500 W CW CO_2 laser which provides the desired output with long term power stability required for laser based nanoparticles synthesis.

2. Theoretical estimation of reduced electric field (*E/N*)

Theoretical estimation of E/N in the positive column requires the knowledge of individual ionization rates of CO_2, N_2 and He gases. These ionization rates along with the mobility of positive ions (CO_2^+, N_2^+, He^+) in the gas mixture determines the electron production term (PT, left hand side of Eq. (3)). Similarly, the loss term (LT, right hand side of Eq. (3)) requires value of electron temperature under given operating conditions. The E/N value in the discharge is found by iterating the values of E/N and finding the PT and LT terms in Eq. (3). The flow chart to calculate sustaining E/N in the positive column is presented in Fig. 3. The flow chart begins with a chosen value of E/N. The electric field E in the positive column is then found by multiplying the selected E/N value with the neutral number density of gas N_0 at the average gas temperature T_g corresponding to input power density Q_{in} in the positive column of the glow discharge. The input power density Q_{in} in the glow discharge is expressed as;