LOW-TEMPERATURE PLASMA

RF Discharge in CO$_2$ Laser Mixtures at Moderate Pressures


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Abstract—The voltage–power characteristics and spatial structure of an RF discharge in the mixtures of CO$_2$ and N$_2$ molecular gases with He at total pressures of tens of torr are studied. One-dimensional numerical simulations of an RF discharge are carried out within two approaches: (i) the distribution function and the related kinetic coefficients are assumed to be functions of the local reduced field, and (ii) the kinetic coefficients are functions of the electron mean energy, which is calculated with allowance for both electron heat conduction and diffusion. The latter approach is shown to better describe the existing experimental dependence of the discharge voltage and the phase shift between the discharge current and voltage on the driving power. © 2002 MAIK “Nauka/Interperiodica”.

1. INTRODUCTION

Recently, great progress has been achieved in creating CO$_2$ and CO capillary and slab lasers excited by a capacitive transverse RF discharge (see, e.g., [1–3]). In these lasers, the gas mixtures are cooled via electrodes, to which an RF driving voltage is applied. The properties of this type of discharge were investigated experimentally in [4–8]. The discharge operated in capillaries (used in laser devices [4]), plasma slabs [5, 8], and specially designed cells [6, 7]. In particular, the dependences of the discharge voltage and the phase shift between the discharge voltage and current on the discharge current and the driving power were studied in [6, 7]. To attain a high lasing power and efficiency, it is necessary that the gas mixture pressure $p$ be tens of torr, the driving field frequency $f$ be in the range from tens to hundreds of megahertz, and the interelectrode spacing be $d = 0.1–0.25$ cm [1, 2]. Under these conditions, numerical simulations of an RF discharge are rather complicated because of the large value of the $pd$ parameter. Early studies on numerical simulations of an RF discharge were reviewed in [9]. Analytical models describe an RF discharge only qualitatively [10]. In a number of papers, the characteristics of an RF discharge were calculated numerically (see, e.g., [5, 11, 12] and review [9]). However, no comparative studies of the results of numerical simulations and available experimental data have been made.

It is generally believed that, at elevated gas pressures, the nonlocal character of the electron energy distribution function can be neglected throughout the entire volume, including the sheaths. However, a true threshold pressure for the applicability of the local model, as well as the dependence of this pressure on various parameters (gas composition, discharge power, etc.), is still unknown.

The aim of this study is to investigate this problem under conditions typical of the active medium of a slab CO$_2$ laser.

To this end, numerical simulations are performed using two different one-dimensional models of an RF discharge. Both of them include Poisson’s equation for the electric field, transport equations for electrons and positive and negative ions, and the heat conduction equation for the gas temperature in the discharge gap. In the first model (referred to as local), the rates of electron production and loss and the electron transport coefficients are assumed to be functions of the local value of the reduced electric field $E/N$ (where $E$ is the electric field and $N$ is the density of neutral particles). The local model is identical to the model of [11]. In the second model (referred to as nonlocal), described in detail in [9], the rates of electron production and loss and the transport coefficients are assumed to be functions of the electron mean energy. To determine this energy, the balance equation with allowance for electron heat conduction and diffusion is solved. Hence, possible deviations of the electron mean energy and the accompanying plasma characteristics from those determined by the local electric field are taken into account.

2. EXPERIMENTAL SETUP

The rms voltage is measured directly at the CO$_2$ laser electrodes, which are the same as those used in experiments on optimizing the laser parameters (see [13] and references therein). The discharge gap dimensions are $d = 0.2$ cm, $a = 1.5$ cm, and $L = 37$ cm. A slab is formed by gold-coated copper electrodes and side
walls made from aluminum oxide. A set of matching coils is connected in parallel to the electrodes to ensure both a homogeneous electric field along the electrodes and the resonant matching to the power supply. One electrode is grounded, whereas the other is connected to a 100-MHz voltage source. A CO$_2$ : N$_2$ : He = 1 : 1.5 : 12 + 5% Xe gas mixture is used.

The measurements were carried out using a Tektronix TDS 640A oscillograph with a bandwidth of 500 MHz and a high-voltage probe with an input impedance of 20 MΩ, 2 pF and an output impedance of 1 MΩ. To measure the RF voltage, the probe was calibrated in the frequency range of interest by measuring the voltage drop across a 50-[OMEGA] load resistor connected to the RF generator. In the absence of the reflected signal (the incident and reflected RF powers were measured with a Werlatone C2310 directional coupler), all the power is dissipated in the load and the voltage is $V = \sqrt{wR}$, where $w$ is the power dissipated in the load and $R$ is the load resistance. Based on these measurements, the voltage calibration factor was determined.

3. DISCHARGE MODEL

Following [11], when simulating an RF discharge, we took into account one positive and one negative ion species. The continuity equations for these components were solved together with the continuity equation for the electron density and Poisson’s equation for the electric field. The continuity equations took into account both drift and diffusion. The gas temperature was determined from the time-independent heat conduction equation.

Note that the results of numerical simulations of the discharge parameters (especially the phase shift between the discharge current and voltage) are sensitive to the exact value of the thermal conductivity of the gas mixture, which was determined from the thermal conductivities of the individual components by the procedure described in [14]. The thermal conductivities of the individual components and their temperature dependences were taken from [15].

When simulating an RF discharge, we used the local and nonlocal models. In the local model, the rates of ionization and electron attachment, the electron mobility, and the coefficients of electron recombinations and diffusion depend only on the local E/N value, which is the case of [11].

Under the conditions of interest, the rate of electron momentum relaxation in the plasma of an RF discharge in a CO$_2$ : N$_2$ : He mixture is two orders of magnitude higher than the frequency of the driving field. Near the electrodes, the rate of electron energy relaxation is also higher than the frequency of the driving field; however, in the middle of the discharge gap, they can be of the same order of magnitude. Generally, the electron energy relaxation length is $10^{-3}$ cm. It will be shown below that the thickness of the sheaths (where the electric field sharply increases, whereas the electron density decreases) is $\sim 10^{-2}$ cm. Taking into account the non-steady and nonlocal character of the kinetic coefficients requires solving the space- and time-dependent Boltzmann equation, which is a rather complicated problem (in [16], such a problem was solved for the case of pure He). Although the electron energy distribution function is different from the Maxwellian one, it is possible to introduce the electron mean energy, regarding it as the main characteristic of the distribution function. We assume that all the coefficients depend only on this mean energy, as was done in [9]. In this case, in order to find the electron mean energy, it is necessary to solve the equation for this energy with allowance for electron heat conduction. At every instant, the electron mean energy is determined at any point of the interelectrode gap. Then, the ionization and attachment rate constants are calculated as functions of this energy (these functions were determined beforehand by numerically solving the Boltzmann equation for the electron energy distribution function). The transport coefficients, which are used to solve the time-dependent equation for the electron mean energy and the continuity equations, are also found. This nonlocal model was previously used in modeling an RF discharge in a He : Ar : Xe mixture [17].

The equations are supplemented with the relevant boundary and initial conditions. The discharge voltage is derived from a given RF power. To solve the set of equations numerically, the finite-difference scheme, which was proposed in [18] for describing processes in semiconductor devices and first used in [19] for simulating an RF discharge, is applied.

In numerical simulations, we used a spatial mesh with a nonuniform cell size, which decreased when approaching the electrodes. In general, the number of such spatial cells was about 100. A steady state was reached after several thousands of RF cycles, which took about 10 h of processing time of an IBM-compatible PC with a Pentium III-733 processor.

4. RESULTS AND DISCUSSION

Only a few experimental studies of a planar RF discharge in CO$_2$-containing mixtures used in CO$_2$ lasers are available in the literature.

In [8], measurements of the rms discharge voltage were carried out at lower specific driving powers and in a gas mixture (CO$_2$ : N$_2$ : He : Xe = 1 : 1 : 3 : 0.25) with a higher content of molecular gases than in our study. The results of numerical simulations with the use of the above two models together with the experimental data from [8] are shown in Fig. 1. At low specific powers, both models provide similar results. As the driving power increases, the nonlocal model shows a more rapid increase in the rms discharge voltage and better matches the experimental data than the local model.
In [6, 7], an RF discharge ran in the specially designed cells—discs with diameters $D = 3$ and 1.7 cm and interelectrode spacing of 0.25 and 0.175 cm, respectively. In addition to the rms discharge voltage, the phase shift between the discharge current and voltage as a function of the discharge input power was also measured. The measurements were performed in a wide pressure range $p = 20–130$ torr in the gas mixture $\text{CO}_2 : \text{N}_2 : \text{He} : \text{Xe} = 19 : 19 : 57 : 5$. Note that, in [7], the measurements were carried out with a refined technique and the measured phase shift was lower than in [6].

To find the phase shift between the discharge current and voltage, two methods for processing simulation results were used: spectral decomposition and the least squares method. Since, in simulations, the voltage at the electrodes was specified as sinusoid (its amplitude was determined by the given driving power), there were high-frequency harmonics in the calculated discharge current. An example of the simulated discharge current is shown in Fig. 2. The spectral decomposition was carried out with the help of the fast Fourier transform [20] and a numerical code kindly provided by N.N. Elkin. Based on the spectral decomposition results, the phase shift between the discharge voltage and the fundamental harmonic of the current was determined. The nonlinear distortion factor, which was determined as the ratio of the sum of the squared amplitudes of higher current harmonics to the squared amplitude of the fundamental harmonic, is $\sim 1\%$. In the least squares method, the discharge current was approximated by the function $J_d = J_{d0}\sin(2\pi f t + \phi)$, where $f$ is the known frequency of the driving field. As a result, the amplitude of the discharge current density $J_{d0}$ and the phase shift $\phi$ were determined. The difference between the phase shifts determined by the two different methods did not exceed one-tenth of a degree.

Figure 3a presents the measured [7] and simulated rms discharge voltages versus the driving power for different gas mixture pressures. The solid and dashed lines show the simulation results obtained with the nonlocal and local models, respectively. It is seen that the nonlocal model better describes the experimental data, especially at reduced pressures. The difference between the results of the alternative models is largest at a pressure of 20 torr and, then, decreases with increasing pressure. Figure 3b presents the phase shift between the discharge voltage and current. The symbols show the experimental data from [7], and the curves show the simulation results obtained with the nonlocal (solid line) and local (dashed line) models. With the exception of the lowest pressure range (near 20 torr), the nonlocal model fairly well describes the experimental data from [7]. The local model predicts a phase shift much lower than the measured one.

We measured the rms discharge voltage as a function of the discharge input power in the $\text{CO}_2 : \text{N}_2 : \text{He} = 1 : 1.5 : 12 + 5\% \text{ Xe}$ gas mixture with a higher helium content at two mixture pressures: 50 and 120 torr. The experimental and simulation results are shown in Fig. 4. As was expected, the difference between the rms discharge voltages calculated using the local (curves 1, 2) and nonlocal ($1'$, $2'$) models decreases as the gas mixture pressure increases. It is notable that, under the given conditions, the local model predicts an increase in the rms discharge voltage with gas pressure (cf. curves $1'$, $2'$) at a constant driving power, which disagrees with the experimental data. The nonlocal model predicts a decrease in the rms discharge voltage with increasing gas mixture pressure (cf. curves 1, 2), which is in agreement with the experiment (see, e.g., review
This decrease is related to the fact that the rms discharge voltage is combined from the voltage drops across the positive column and electrode sheaths [10]. The rms reduced field \( \frac{E}{N} \) in the middle of the discharge gap is determined by the balance between the electron production and loss and, according to numerical simulations (Fig. 6), depends slightly on the pressure and specific driving power; therefore, \( E \) increases with pressure \( p \). Consequently, at a constant specific driving power \( W =JE \), the discharge current density \( J \) decreases. Since the continuity of the total discharge current at the electrodes is ensured by the displacement current, the decrease in \( J \) leads to a reduction in \( \partial E_{el}/\partial t = J \) and a subsequent decrease in both the electric field \( E_{el} \) in the sheath and voltage drop across the sheath. Hence, the quantity \( \frac{U_{RMS}}{H_{11229}} \) decreases with pressure if the second term in the radicand dominates. In the opposite case, \( U_{RMS} \) increases with pressure. Our calculations confirm this consideration.

In experiments [6, 7], the data processing made it possible to separate the voltage drops across the plasma and the sheaths; for this reason, further numerical simulations are carried out for the conditions of [7]. The reduced electric field \( \frac{E}{N} \) is an important parameter that determines both the energy fraction spent on the excitation of vibrational levels and the related efficiency of the lasers based on vibrational–rotational transitions. The profiles of the rms \( \frac{E}{N} \) are shown in Figs. 5a–5d for different driving powers and gas pressures. It is seen that, at a pressure of 20 torr, the local model (Fig. 5a) predicts narrower sheaths and a more pronounced sheath shrinking with increasing driving power than the nonlocal model (Fig. 5b). At a pressure of 130 torr, both models show similar \( \frac{E}{N} \) profiles (Figs. 5c, 5d).

As was discussed above and is seen in Fig. 5, the value of \( E/N \) in the middle of the discharge gap changes slightly with increasing driving power. The increase in the discharge input power leads to an increase in the electron density. As the gas mixture pressure decreases, the electron losses due to ambipolar diffusion start to dominate in the electron balance in the middle of the discharge gap. The dependence of the rms reduced electric field in the middle of the discharge gap on the electron density is shown in Fig. 6. At pressures of 70–130 torr, the difference between the \( E/N \) values calcu-
lated using the alternative models is small. As the pressure decreases to 20 torr, this difference becomes significant. As the pressure increases from 20 to 130 torr, the \( E/N \) value in the middle of the discharge gap decreases from \( 6 \times 10^{-16} \) to \( 2.6 \times 10^{-16} \) V cm\(^2\). The local model predicts that \( E/N \) decreases with increasing electron density, whereas, according to the nonlocal model, the reduced field increases and this increase becomes less pronounced with increasing gas pressure.

The small signal gain profiles in molecular lasers depend on the profiles of the specific driving power. Figure 7 shows the profiles of the specific driving power \( W_{\text{total}} \) for different averaged specific driving powers \( \langle W \rangle \) and gas mixture pressures \( p \). As is the case of the reduced electric field, the \( W_{\text{total}} \) profiles calculated using the local and nonlocal models differ greatly at a gas mixture pressure of 20 torr (Figs. 7a, 7b) and are similar at a pressure of 130 torr (Figs. 7c, 7d). Simulations show that the corresponding sheaths occur in the profiles of the electron, positive ion, and negative ion densities. Note that, at a pressure of 20 torr and an average specific driving power of \( \langle W \rangle = 26 \) W/cm\(^3\), the local model predicts a significant increase in the specific driving power near the electrodes (Fig. 7a, curve 5). This increase is related to the increase in the positive ion current. The profiles of the rms densities of the conduction current, positive and negative ion currents, and displacement current calculated using the local and nonlocal models for a pressure of 20 torr and \( \langle W \rangle = 26 \) W/cm\(^3\) are shown in Figs. 8a and 8b, respectively. In the middle of the discharge gap, the main contribution to the total current is provided by the electrons (Figs. 8a, 8b, curves 1), whereas near the electrodes, the displacement current prevails (Figs. 8a, 8b, curves 2). As the driving power increases, the electric field
near the electrodes also increases, thus ensuring a higher displacement current, which is proportional to \(\frac{\partial E}{\partial t}\). The increase in the \(E/N\) near the electrodes leads to an increase in the ionization rate and the positive ion density; as a result, the fraction of the positive ion current in the total current becomes higher (Fig. 8a, curve 3). Simulations predict that the fraction of the negative ion current is small (Figs. 8a, 8b, curves 4).

In [6], a method for separating out the voltage drops across the plasma and sheaths from the discharge voltage was proposed. The method is based on the equivalent circuit of an RF discharge, including the sheath capacitance connected in series with the parallel connection of the plasma active resistance and the discharge gap capacitance, which is determined by the discharge geometry. Given the driving power, the discharge voltage, and the phase shift between the current and voltage, we can determine the rms voltage drops across the sheaths and plasma [6]. Using that procedure and based on the results of simulations, we determined
these voltage drops, which are shown in Fig. 9 together with the experimental data (symbols) from [7]. In both the experiment and simulations, the voltage drop across the plasma slightly depends on the discharge input power (Fig. 9a). Both the local and nonlocal models give close results; however, the experimental data are somewhat lower. The sheath voltages calculated using the nonlocal model (Fig. 9b, solid lines) agree better with the experimental data than those obtained with the local model (Fig. 9b, dashed lines). Based on these results, the capacitance and thickness of the sheaths can be determined. This method for determining the sheath thickness is more suitable than the techniques based on the profiles of the rms reduced electric field, the profiles of the electron density averaged over the RF period, etc., because it does not require any extra criteria. The sheath thickness determined from the results of simulations by the nonlocal model agrees satisfactorily with the experimental data from [7]. Note that the local model underestimates the sheath thickness by a factor of 1.5–2.

5. CONCLUSION

A comparison of the results of numerical simulations by the local and nonlocal models with the experimental data from both the present study and the literature has shown that the nonlocal model better describes the dependences of the discharge voltage and the phase shift between the discharge current and voltage on the driving power in a wide pressure range. In particular, the nonlocal model predicts a decrease in the discharge voltage with increasing gas pressure at a constant driving power, which agrees with the experimental data, whereas the local model predicts the opposite behavior.

On the whole, the nonlocal model satisfactorily describes the dependences of the discharge voltage, the phase shift between the current and voltage, and the voltage drops across the plasma and electrode sheaths on the discharge input power.

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