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EXCITATION OF $^1\Sigma^+_u$ and $^1\Pi_u$ STATES AND IONIZATION OF CO_2 IN DC ELECTRIC FIELD

VIOLETA V. STANKOVIĆ[1], MIRJANA M. VOJNOVIĆ[1],
MIROSLAV M. RISTIĆ[2], SAVA M. D. GALIJAŠ[1] and GORAN B. POPARIĆ[1]

[1]*University of Belgrade, Faculty of Physics, Studentski Trg 12, P.O.Box 44, 11000 Belgrade, Serbia*

[2]*University of Belgrade, Faculty of Physical Chemistry, Studentski Trg 12, P.O.Box 47, 11000 Belgrade, Serbia*

Email violeta.stankovic@ff.bg.ac.rs

Abstract. The topic of this research are the rate coefficients for formation of CO_2 molecules ions formed as a result of collisions between electrons and CO_2 gas molecules. For rates calculation we used non-equilibrium electron energy distribution function obtained by a Monte Carlo simulation in the homogenous external electric field. The calculations are performed for reduced electric field values, E/N, in the range from 20 Td to 1000 Td.

1. INTRODUCTION

CO_2 molecules are currently the research topic by many research communities since the electron interaction with CO_2 molecules is very important in terms of natural phenomena as well as in plasma devices and laser technology. Today the most common natural phenomenon is the greenhouse effects, for which the CO_2 molecule is largely responsible, since it is an essential part of the Earth's atmosphere composition. Also knowledge of energy transfer in the atmosphere of Mars and Venus is increased by the fact that electrons are cooling in process of collision with CO_2 molecules. In order to model all mentioned phenomena, it is necessary to know the probabilities for the involved processes as well as the rate coefficients of them. Electron ionization is a crucial process for maintaining plasma in discharge devices and is also one of the process by which CO_2 is activated. Ionization of CO_2 molecules provides a multitude of ionic species where positive and negative ions are important for plasma maintenance.

CO_2 molecule has already been the subject of research by our group in terms of non- equilibrium rate coefficients. The calculations of them had done by using a

Monte Carlo simulation of electron transport trough CO_2 gas in the presence of DC electric field. Calculations of the rate coefficients for vibrational excitation of CO_2 vs. E/N values, ranging only up to 150 Td, had been performed (see Poparić et al. 2010). The aim of this paper is to provide database of rate coefficients for many ways of obtaining CO_2 ions caused by the movement of electrons under the influence of an external electric field. Such a data set enables the application of modeled plasmas.

2. MONTE CARLO METHOD

The results presented in this paper were obtained using the Monte Carlo simulation. Simulation involves monitoring the transport of an ensemble of electrons (10^7). Electrons are moving under the influence of the external homogenous DC electric field in the infinite space filled with neutral CO_2 gas (pressure 5 Torr). Each electron is observed and monitored individually for a given set of input parameters. At the initial moment electrons are characterized by the nonzero kinetic energy which is seated around the expected mean electron energy as input parameter. The following differential equation describes the motion of each electron in mentioned ensemble:

$$m\frac{d^2\boldsymbol{r}}{dt^2} = e(\boldsymbol{E}) \tag{1}$$

In this equation $\boldsymbol{r}$ is the radius vector of the electron, m and e are the electron`s mass and charge and $\boldsymbol{E}$ is the electric field. The CO_2 molecules are assumed to be at zero temperature at their vibrational, rotational and electronic ground states. The possible collision event is determined by the random number which is weighted by probability of the certain event. Probability of possible elastic or inelastic event is calculated by using the integral cross section which the program contains as input data folder and interpolated for the corresponding kinetic energy. When equilibrium is established between the energy transmitted by the electrons to the neutrals and the energy which electron is receive by the electric field, the electron energy distribution function is sampled in equidistant time steps.

Our cross section (CS) database contains CSs for elastic and nonelastic collision processes, mostly originating from measurements, while some are determined by theoretical models.

To validate the simulation code, we performed tests by comparing the electron transport parameters obtained by the simulation with benchmark calculations found in literature for different model gases. These are the Reid model gas (see White et al. 1999) for conservative collision processes and the modified Ness-Robson model gas (see Nolan et al. 1997) for nonconservative collision processes (ionization and electron attachment). For more details about Monte Carlo simulation code and our cross section database we refer to reference Vojnović at al. 2019.

3. RESULTS

After the EEDF is sampled for certain parameters (E_r/N), it is used to calculate the value of the electronic excitation rate at a certain moment of the external electric DC field influence. The calculation is performed by the following equation:

$$K(\bar{\varepsilon}_t) = \sqrt{\frac{2}{m}} \int_{\varepsilon_{th}}^{\infty} \sigma(\varepsilon)\sqrt{\varepsilon}\, f_\varepsilon(\bar{\varepsilon}_t, \varepsilon) d\varepsilon \qquad (2)$$

where $\sigma(\varepsilon)$ is the cross section for the certain process and ε_{th} is the treshold energy for that process.

In Figure 1 the partial ionization rate coefficients of the formed several ionic species of CO_2 gas are represented, depending on the reduced electric field, E_r/N, in the range form 20 Td to 1000 Td.

Also, in Figure 2, one can see the rate coefficients for excitation of the $^1\Sigma^+_u$ and rate $^1\Pi_u$ electronic states of CO_2 gas calculated in the condition of zero magnetic field and reduced electric field, E_r/N, in the range from 20 Td to 1000 Td.

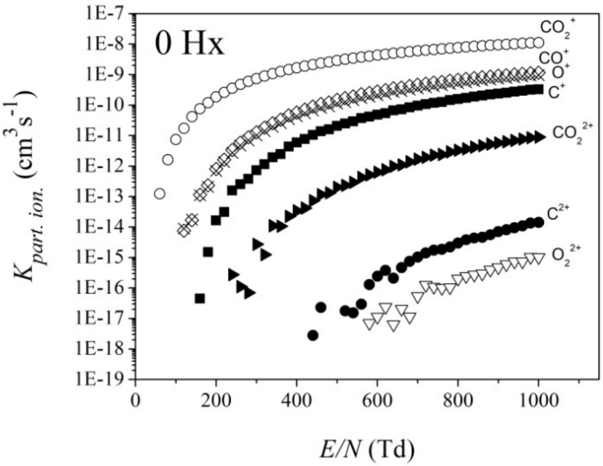

Figure 1: Partial ionization rate coefficients of the CO_2 gas vs. reduced electric field, E/N, in the range from 20 Td to 1000 Td and for zero magnetic field.

In addition to the fact that the pure CO_2 gas after ionization by electrons becomes a complex mixture of the shown ionic species and neutrals, we can see that the highest rate coefficient is for formation of CO_2^+ ion almost in the whole applied range of reduced electric field. It is expected because formation of the CO_2^+ ion is the most probable formation by electron impact ionization, in relation to formation of other ionization channels. The formation of other ionic species requires the application of a more intense electric field, but the rate coefficient of electron impact ionization for these species is certainly lower.

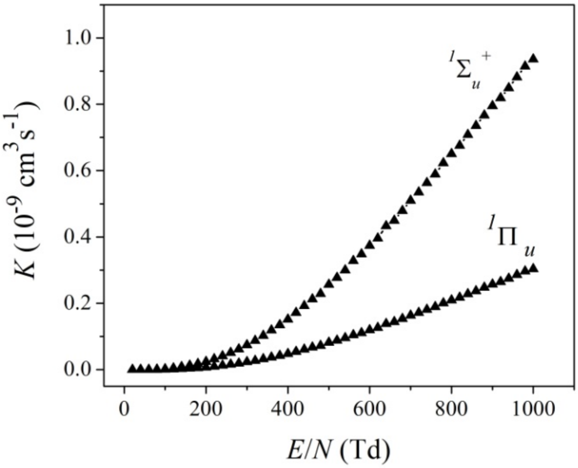

Figure 2: Rate coefficients of the $^1\Sigma^+_u$ and $^1\Pi_u$ state excitations of CO_2 gas vs. reduced electric field, E/N, in the range from 20 Td to 1000 Td and for zero magnetic field.

In the figure 2 one can see the rate coefficients values of the $^1\Sigma^+_u$ and $^1\Pi_u$ electronic state follow the growth of the applied electric field strength. The rate coefficient of $^1\Sigma^+_u$ electronic state increases almost exponentially with increasing strength of the applied electric field, where it can be noticed that the value of the its rate coefficient is the highest at the maximum applied field strength (1000 Td). Both electronic states can be said to have a uniform value of the ionization rate coefficient in the initial part of the curve in figure 2, approximately in the range from 0 Td to 200 Td, after which a slightly weaker increase of excitation rate coefficient of $^1\Pi_u$ electronic state is observed.

The presented dataset is expected to be helpful for understanding the processes of DC CO_2 plasma which also directly affects the quality modeling of this plasma type.

Acknowledgments

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