

Electron kinetics in CO₂/CO mixtures

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This contribution addresses the electron kinetics in CO₂/CO mixtures, in order to evaluate the influence of the CO created as a result of CO₂ dissociation in a plasma discharge. It is shown that vibrational excitation of CO has a significant role in shaping the electron energy distribution function (EEDF) and that CO influences in a complex way the low-energy region of the EEDF, of significant importance to control the energy input into the CO₂ asymmetric stretching vibration mode.

Carbon dioxide (CO₂) is an important trace gas in Earth's atmosphere, as a major cause of the climate change, and is the main component of the atmospheres of Mars and Venus. The use of plasmas for CO₂ dissociation is a hot topic nowadays, being discussed in different contexts, from CO₂ gas mixtures in Earth for the production of solar fuels [1] to Mars low-temperature and low-pressure atmospheric conditions for oxygen production [2]. Non-equilibrium plasmas can promote CO₂ dissociation by direct electron impact or through vibrational excitation [3]. The study of electron kinetics is essential, allowing to understand how the energy gained by the electrons is transferred to the different heavy-particles

The products of dissociation of carbon dioxide are CO and atomic oxygen. Even small concentrations of these gases can change the behaviour of the discharge [4]. Herein we discuss the influence of CO on the electron kinetics of a CO₂ discharge. To this purpose, we use the Boltzmann solver of the LisbOn KInetics simulation tool (LoKI-B) [5] to calculate the electron energy distribution function (EEDF), transport coefficients, reaction rate coefficients and power balance in CO-CO₂ mixtures. We focus on three different CO-CO₂ mixtures, from 100% CO to small amounts of carbon monoxide admixture, and two values of the reduced electric field, E/N , of 10 and 100 Td.

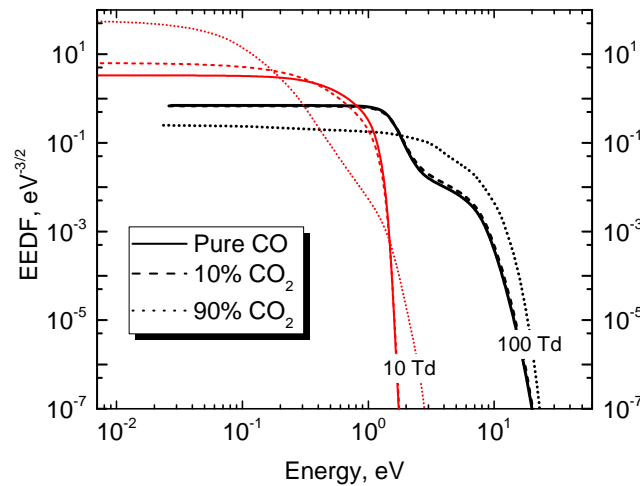


Fig. 1: EEDFs versus electron energy for $E/N = 10$ and 100 Td.

Figure 1 reports the EEDFs calculated for the conditions under study. The addition of small concentrations of CO₂ introduces only small changes in the shape of EEDF. For the pure CO and 10% CO₂ cases, we can notice a strong depletion of the EEDF around 1-2 eV. This is due to the resonant part of the vibrational cross sections of CO, which makes it difficult for electrons to reach higher energies. At low E/N the role of electronic excitation in shaping the EEDF is negligible, but it starts to be noticeable

at higher reduced fields, with the appearance of second depletion region at 7-8 eV. The outcome is an opposite behaviour of the EEDF with CO₂ addition in the electron energy region $u < 0.2$ eV for low and high E/N . In particular, for large amounts of CO the EEDF in this region is more/less populated at low/high E/N .

CO₂ is quite a complex molecule, with three vibrational modes. The asymmetric stretching mode has a threshold at 0.17 eV and is believed to contribute to an efficient dissociation of CO₂ through the vibration-vibration (V-V) ladder-climbing mechanism [6]. Slow electrons are therefore responsible for the input of energy into this mode and induce the V-V up-pumping. Figure 2 details the vibrational energy transfer pathways in CO₂ for two mixture compositions, 10% and 90% of CO₂. The rate coefficients of excitation of the asymmetric stretching mode are a manifestation of the changes in the EEDF discussed above. This figure reveals that finding the ideal working conditions to enhance CO₂ dissociation is not straightforward, as the dissociation products modify the ideal reduced fields for discharge operation, implying that the optimisation of a CO₂ plasma must take into account the kinetics of the formed CO in some detail, as also pointed out in [4].

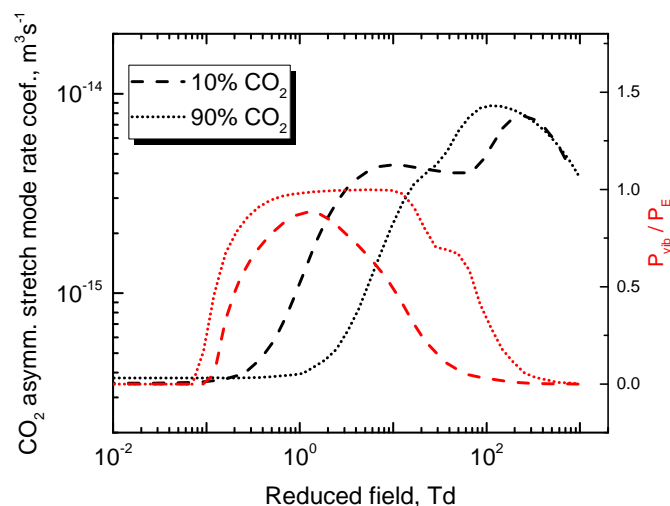


Fig. 2: Rate coefficient of excitation of the first level in the asymmetric stretching mode (black, left axis) and fractional power dissipated by electrons onto vibrational excitation of CO₂ (red, right axis), as a function of E/N .

Acknowledgments

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