Preferred main topic: Modeling and Diagnostics

Abstract title: N_2 influence on the vibrational distribution of the asymmetric level of CO_2 in non-thermal plasmas

Authors: T. Silva (1), M. Grofulovic (1), A. S. Morillo-Candas (2), O. Guaitella (2), V. Guerra (1) and L. Terraz (1)

Affiliations:

- (1) Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Portugal
- (2) LPP, Ecole Polytechnique, UPMC, Université Paris Sud-11, CNRS, Palaiseau, France

Abstract:

DC pulsed discharges in CO₂-N₂ plasmas ignited at room temperature, pressures between 1 and 5 Torr and currents between 20 and 50 mA, show an increase of CO₂ dissociation when molecular nitrogen is present [1]. In this case, dissociation is assumed to be obtained partly from highly vibrating molecule collisions, as well as from direct electronic impact. The former process is enhanced by strong non-Boltzmann distributions of the vibration levels, typical from cold plasmas. The CO₂ molecule possess 3 vibrational modes, namely the symmetric v_1 , the bending v_2^{12} and the asymmetric v_3 , represented following Herzberg's notation as $CO_2(v_1, v_2^{12}, v_3)$. Molecular nitrogen is known for having its lower vibration energy levels almost equal to those of $CO_2(00^0v_3)$, allowing N_2 to easily exchange vibration quanta with the asymmetric mode of CO_2 . Hence the possibility that previously excited molecular nitrogen injected in a CO₂ cold plasma can favor CO₂ dissociation. In order to investigate the kinetics of such plasmas, a self-consistent model is developed, able to reproduce time-resolved experimental results for the populations of several CO₂ vibrational levels and to quantify the relative importance of all the processes involved in CO₂ dissociation. The model accounts for about 70 vibration levels for CO₂ and 10 levels for N₂, where all the species are at the ground electronic state. It includes reaction datasets for the vibrationtranslation energy exchanges (V-T), vibration-vibration exchanges (V-V) and excitation by direct electron impact (e-V) in mixtures of CO_2 -N₂, extending the work in pure CO₂ from [2]. The e-V processes are derived from the LisbOn KInetics Boltzmann code (LoKI-B). The overall good agreement between the model predictions and the experimental results provides a validation of the current kinetic scheme. Some discrepancies remain, which can however be justified by the influence in the kinetics of some species not considered in the current model, namely CO, O and O₂. The present simulations strongly suggest the possibility of using previously excited N₂ to assist CO₂ dissociation.

References:

[1] M. Grofulović, B. L. M. Klarenaar, O. Guaitella, V. Guerra and R. Engeln, *Submitted to PSST*, 2019

[2] T. Silva, M. Grofulović, L. Terraz, C. D. Pintassilgo, and V. Guerra, *Journal of Physics D: Applied Physics*, 2018

Acknowledgment:

This work was partially supported by the Portuguese FCT, under Projects UID/FIS/50010/2013, PTDC/FISPLA/1420/2014 (PREMiERE) and PTDC/FISPLA/1243/2014 (KITPLASMEBA). V. Guerra was partially supported by LABEX Plas@par under the project ANR-11-IDEX-0004-02. We are indebted to A. S. Morillo-Candas, B. Klarenaar and O. Guaitella for sharing their experimental data and for many and invaluable discussions.