# PhD Open Days

2nd edition!

16 - 17 MAY / SALÃO NOBRE


# Electron-neutral scattering cross sections for $CO_2$

Advanced Program in Plasma Science and Engineering - APPLAuSE


Marija Grofulović (marija.grofulovic@tecnico.ulisboa.pt), GEDG-IPFN/IST


## Introduction

Conversion of carbon dioxide ($CO_2$) using plasma technology is considered a great scientific challenge. A detailed understanding of the first step in the process – the $CO_2$ dissociation by plasma – is essential for its control and optimization [1]. To address this problem, a comprehensive knowledge of the electron kinetics is required. Accordingly, a reliable quantification of electron-impact cross sections and a critical evaluation of available dissociation cross sections are needed. This work offers a set of electron–neutral scattering cross sections from ground-state $CO_2$, to be published on the IST-LISBON database with LXCat, and evaluates and recommends cross sections for providing the rate coefficients for electron-impact $CO_2$ dissociation.

## Results and discussion

The proposed swarm-derived complete and consistent set of electron-neutral scattering cross sections from ground-state $CO_2$ includes 17 cross sections.

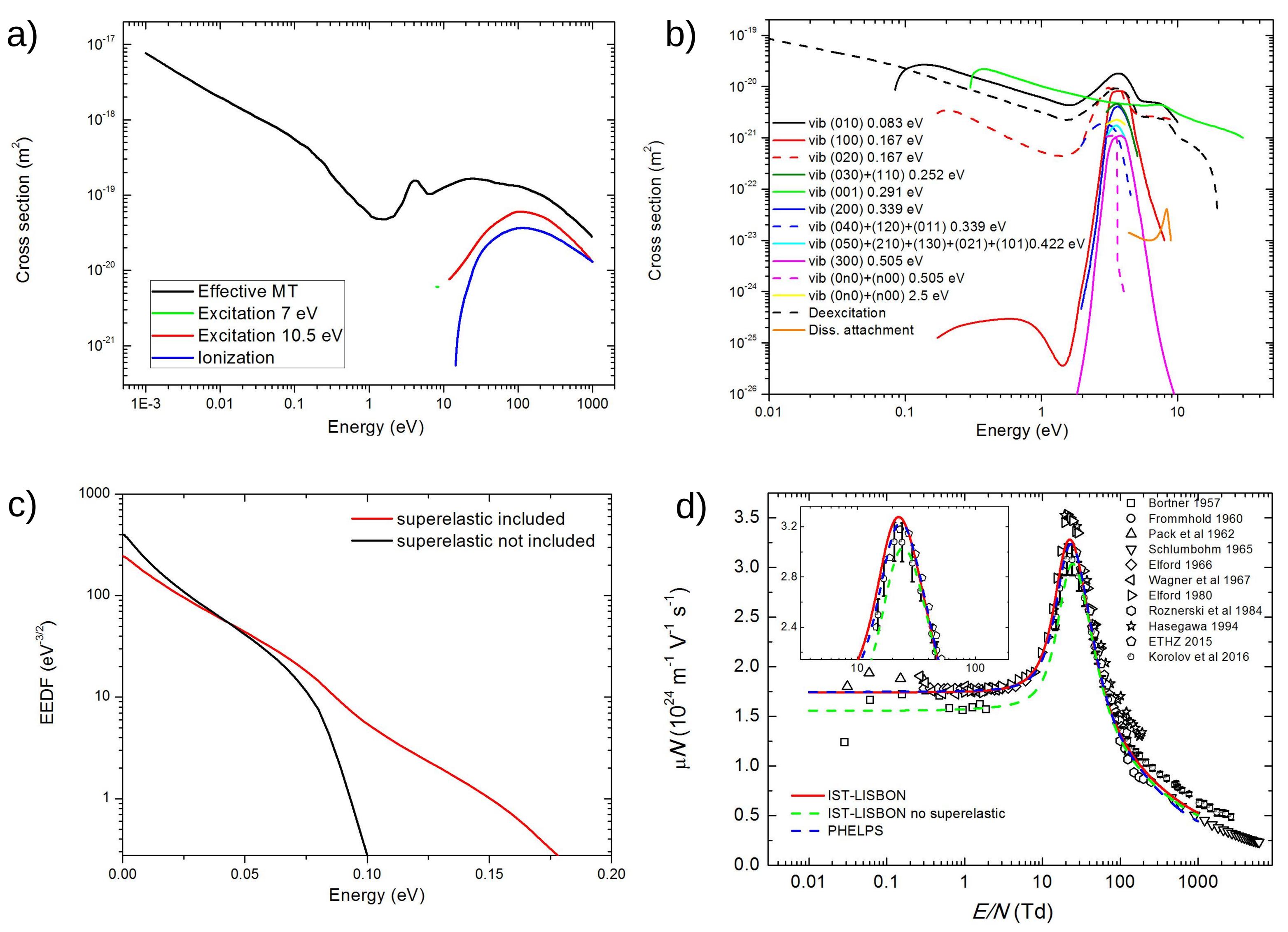


Fig.1. Summary of the proposed $CO_2$ cross section set, as a function of the electron kinetic energy a) and b); EEDF obtained with the proposed set for 1 Td c); measured and calculated reduced electron mobility as a function of the reduced electric field d).

The set was compiled mostly from Phelps [2] and includes the cross sections defined up to 1000 eV, describing dissociative attachment, effective momentum transfer, eight vibrational excitation energy losses (corresponding either to the excitation of individual levels or groups of vibrational levels), superelastic collisions with the $CO_2(010)$ vibrational state, excitation of two groups of electronic states and and ionization (see table 1).

**Table 1.** Summary of the processes considered in the cross section set proposed.

| | Heavy–species products | Configuration of final $CO_2$ state | Threshold [eV] |
|---|---|---|---|
| Effective momentum–transfer | $CO_2(v_0)$ | (000) | |
| Dissociative attachment | $CO+O^-$ | | |
| Vibrational excitation | $CO_2(v_1)$ | (010) | 0.083 |
| Superelastic deexcitation | $CO_2(v_0)$ | (000) | |
| Vibrational excitation | $CO_2(v_{2a})$ | (020) | 0.167 |
| Vibrational excitation | $CO_2(v_{2b})$ | (100) | 0.167 |
| Vibrational excitation | $CO_2(v_3)$ | (030)+(110) | 0.252 |
| Vibrational excitation | $CO_2(v_4)$ | (001) | 0.291 |
| Vibrational excitation | $CO_2(v_{5a})$ | (200) | 0.339 |
| Vibrational excitation | $CO_2(v_{5b})$ | (040)+(120)+(011) | 0.339 |
| Vibrational excitation | $CO_2(v_6)$ | (050)+(210)+(130)+(021)+(101) | 0.442 |
| Vibrational excitation | $CO_2(v_{7a})$ | (300) | 0.505 |
| Vibrational excitation | $CO_2(v_{7b})$ | (0n0)+(n00) | 0.505 |
| Vibrational excitation | $CO_2(v_8)$ | (0n0)+(n00) | 2.500 |
| Electronic excitation | $CO_2(e_1)$ | | 7.0 |
| Electronic excitation | $CO_2(e_1)$ | | 10.5 |
| Total ionization | $CO_2^+$ | | 13.3 |

The cross sections are summarized in Figs. 1a) and b). A small number modifications was made in regard to the original set by Phelps. First, superelastic collisions with the first level of the bending mode were included and should be considered as an integral part of the set. As a matter of fact, due to its low energy threshold (0.08 eV), this level presents a non-negligible population even in thermal conditions and influences the electron kinetics, specially at low values of the reduced electric field. In the original set [2] the electronic excitation with the threshold at 10.5 eV and the ionization cross sections are limited to 100 eV kinetic energy. The cross section corresponding to the aforementioned electronic excitation was extended up to 1000 eV, while the ionization cross section was replaced by the total ionization cross section from [3]. Considering the extension of the inelastic cross section for u > 100 eV, the effective momentum transfer cross section is modified in the same energy region. Finally, the effective momentum transfer cross section was slightly increased for electron energies below 1eV, in order to somehow compensate for the additional gain of energy associated with the superelastic collisions.

When this complete set of cross sections is used as input data in a two-term Boltzmann code it yields calculated swarm parameters in agreement with available swarm measurements, as discussed in [4,5]. The present calculations show that the energy gained in the superelastic process is relevant for low (E/N > 10 Td) reduced electric fields (Fig. 1c, d).

The cross section set presented in this work will be soon available in the IST LISBON database with LXCat (www.lxcat.net). At present, the IST-LISBON database includes complete and consistent sets of electron scattering cross sections for argon, helium, nitrogen, oxygen, hydrogen and methane, concluded by the Group of Gas Discharges and Gaseous Electronics with Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Lisboa, Portugal.

**References**


[1] A. Fridman, Plasma Chemistry, Cambridge University Press, Cambridge, 2008.
[2] J. J. Lowke, A. V. Phelps and B. W. Irwin, J. Appl. Phys. 44 (1973) 466471.
[3] Y. Itikawa, J. Phys. Chem. Ref. 31 (2002) 749-767.
[4] M. Grofulović et al, ESCAMPIG 2016 (submitted).
[5] M. Grofulović, L. L. Alves and V. Guerra, J. Phys. D: Appl. Phys. (submitted)
[6] PHELPS database, www.lxcat.net, retrieved on May, 2015.




Supervisor: Vasco Guerra

APPLAuSE