AP061201

Proceedings of the 6th International Conference on Reactive Plasmas and 23rd Symposium on Plasma Processing

ICRP-6/SPP-23

January 24-27, 2006
Hotel Taikanso
Matsushima/Sendai, Japan

Edited by
Rikizo Hatakeyama and Seiji Samukawa

Sponsored by
The Japan Society of Applied Physics
Cosponsored by
Nagoya Industrial Research Institute
In conjunction with
Nanotechnology Researchers Network Center of Japan nanonet

G-1B-2

Electron scattering on triatomic molecules - the need for data

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In this paper we discuss existing data for electron scattering for triatomic molecules (H_2O, CO_2, N_2O, NO_2, SO_2, OCS) indicating some similarities between targets, giving recommended sets where possible and indicating need for new data.

1. Introduction

Experimental data on electron-scattering cross sections, our understanding of underlying processes and the possibility of translating cross sections into plasma properties is still far from being perfect. The most studied molecule case, N_2 is the best example. In the region of 2 eV a resonant process is present, increasing by two orders of magnitude the vibrational excitation, see [1], still not fully understood by the theory [2]. In nitrogen plasma afterglow, an unexpected yellow zone appears, probably due to presence of molecular excited, optically forbidden states [3]; such states show strong enhancement at the threshold in positron collisions [4] but in electron collisions probably not.

2. Triatomic molecules, beam data

Triatomic molecules, (i) H_2O, (ii) CO_2, N_2O, (iii) NO_2, SO_2, OCS, are or basic importance for (i) biology, (ii) laser technologies and atmospheric chemistry, (iii) atmospheric pollution. Recommended sets of data are available only for some of them [5-7].

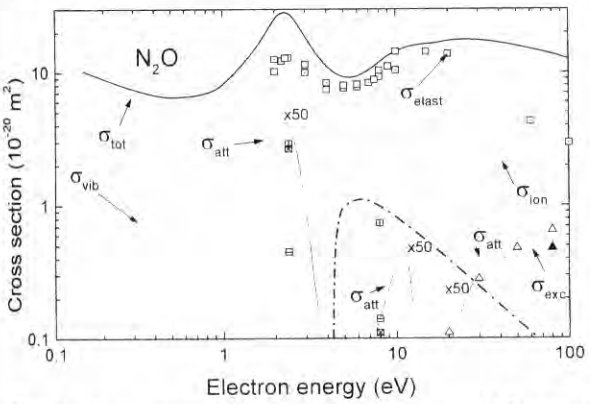

Fig. 1. A recommended set of cross sections used for modeling electron diffusion coefficients in N_2O.

New, accurate measurements of integral cross sections for electron scattering were recenly performed for molecules like CO_2, N_2O, NO_2, OCS, SO_2 (see [8] for an overview). These data comprise elastic and vibrational [9-11], ionization [12,13] and electron attachment [14] processes. The difficulty of partial cross section measurements lies in the necessity of using normalization procedures; the overall determination of integral cross sections hardly exceeds the 20% accuracy. Only ionization shows good agreement among old [15] and new [12, 16] data.

3. Swarm experiments and models

Measurements of electron diffusion coefficients are much simpler that of partial cross sections and are not subject to some inherent errors, like the angular resolution effecting total cross sections. In this method, enlarging (in transverse and longitudinal directions) of the electron packet due to collisions is measured, see for ex. [17]. This effect depends on all scattering processes possible – not only as integral cross sections but also as angular distributions. Therefore, swarm methods can constitute a stringent test on electron-scattering cross section sets.

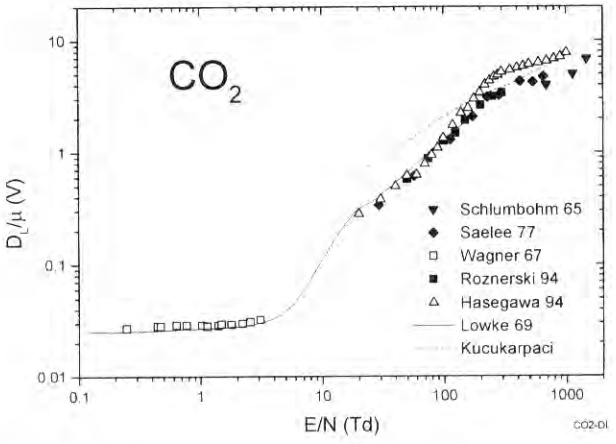

Fig.2. Longitudinal diffusion coefficient for electrons in CO_2. As far as for drift velocities w the data of Hasegawa et al. [18] agree well with Monte Carlo modeling of Kücükarpaci and Lucas [19], with experiment of Saelee et al. [20] and disagree by +20% with the experiment of Roznerski and Leja [21] - the data for D_L/μ of Hasegawa et al. agree with Roznerski and Mechlińska-Drewko [22] but disagree with the Monte Carlo model [19].

However, two steps of numerical procedures have to be employed between the direct experimental data (i.e. measured electron currents) and cross sections. At the first stage, the measured currents to different regions of anode depend on both transverse and longitudinal drift coefficients, and, if charge-changing processes are present like ionization and electron attachment (which is the case of the triatomic molecules considered for intermediate reduced field values) also on them. Different models going through successive approximation steps have been developed for particular drift geometries, in order to account for attachment and ionization processes, see for ex. [22].

Also at the second stage numerical procedures employing Boltzmann equation (Elendif, Bolsig) or Monte Carlo [23] simulations are used. This is an inverse procedure, in which diffusion coefficients are obtained from assumed cross sections sets. As diffusion coefficients average over all possible processes in a wider energy range, in general, it is possible that somewhat different cross section sets produce a good agreement with experimental diffusion coefficients.

3. Partitioning schemes and analogies

Out of the six molecules considered, the only one non-polar is CO_2 (although it has a dipole moment in bending vibrational modes). CO_2 [24], N_2O and OCS [25] show low-energy resonant states, with their position moving to lower energies with rising molecular dipole moment and the amplitude as seen in the total cross section (see fig.3) also rises. Another common feature of these three molecules is a high contribution of vibrational excitation into these resonances, roughly at about 1/3 of the total scattering cross section [8].

Similar analogies regard also other cross sections, like for example dissociative attachment. It is high in "quasi-homonuclear" triatomic molecules, CO_2, N_2O, OCS, NO_2: 0.1%, 0.3%, 0.8% and 0.5% of the total cross section, respectively, see [8]. The bent, NO_2, SO_2 and CS_2 molecules do not show sharp peaks on the total cross sections but the overall amplitude of the cross sections is also high (about 40×10^{-16} cm^2) at 5 eV – probably more than one resonance overlap but are positioned at different energies.

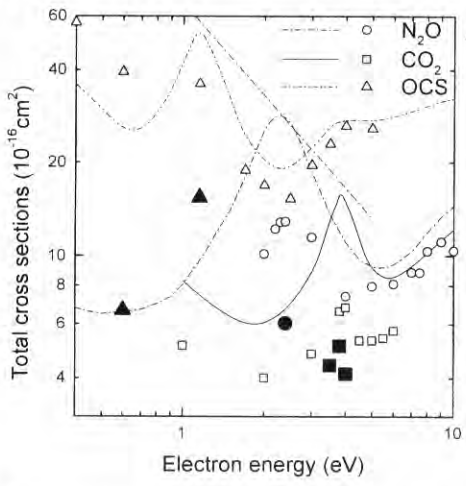

Fig. 3. Analogies in partitioning between elastic and vibrational-excitation channels at low energy "shape" resonances in linear triatomic molecules. The lines are total cross sections, point symbols are elastic integral cross sections from different laboratories, see ref. [8] for references. The data indicate that vibrational excitation can constitute as much as 1/3 of the total cross sections in these resonances. The dash-dot line indicate 1/E dependence of the total cross section peak (from Szmytkowski and collaborators measurements [25]) on collision energy.

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