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MC simulations of nitrogen swarm parameters: comparison of cross-section sets

A. Cenian[a,*], A. Chernukho[b]

[a] Institute of Fluid-Flow Machinery, Polish Academy of Sciences, Fiszera 14, Gdańsk 80-952, Poland
[b] Heat and Mass Transfer Institute, P. Brovki Street 15, Minsk 220072, Belarus

Abstract

The swarm parameters of nitrogen have been reinvestigated using Monte Carlo isotropic method and cross-section (CS) sets compiled by Kochetov (in: L.S. Polak (Ed.), Plasma-Chemical Processes, Nauka, Moscow, pp. 4–43 (1979) (in Russian)), Phelps and Pitchford (Phys. Rev. A 31 (1985) 2932) and Campbell et al. (J. Phys. B 34 (2001) 1185). It was concluded that basing on the existing experimental data and their statistical errors, it is not possible to make a sound recommendation of the CS set—at least for isotropic approximation. Further improvements in CS sets are possible only when the new, more refined experimental data, including longitudinal diffusion coefficient and differential cross section, will be available.

Keywords: Swarm parameters; Nitrogen; MC simulations

1. Introduction

The nitrogen swarm parameters are probably most often calculated and widely discussed due to the fundamental importance of nitrogen molecule, both from theoretical and practical point of view. For example, many papers were devoted to the important issues like the comparison between MC and Boltzmann analyses (see, e.g., Penetrante et al., 1985; Phelps and Pitchford, 1985a) and cross-sections (CS) anisotropy (Phelps and Pitchford, 1985a; Kunhard and Tzeng, 1986).

Lately, Campbell et al. (2001) have revisited the problem using the Ohmori et al. (1988) CS set modified by replacement of old with newly derived integral cross sections for electronic states excitation. A good agreement of calculated and measured swarm parameters was reported in contrast to striking discrepancy with the high-energy results given by Phelps and Pitchford (1985a, b).

However, the calculations using both the Boltzmann equation in two-term approximation (Phelps, 2002) and isotropic MC simulation (Cenian et al., 2002) did not confirm the large differences in swarm parameter values for CS sets CO-CS (Campbell et al., 2001) and P&P-CS (Phelps and Pitchford, 1985b). It was found that the conclusions of Campbell et al. (2001) regarding the usefulness of the P&P-CS set for electron transport calculations were based on a misleading comparison. The swarm parameters calculated by Phelps and Pitchford (1985a) for a pulsed Townsend (PT) experiment were related to the experimental (Wedding et al., 1985; Roznerski, 1996) and the Monte Carlo simulation (Campbell et al., 2001) results for the time-of-flight technique (TOF).

In this paper, we present more thorough analyses of swarm parameters at high E/N values calculated using the CS sets used by Campbell et al. (2001), Phelps and Pitchford (1985a) and Kochetov et al. (1979) using the same isotropic MC analyses as proposed by Campbell et al. (2001). The work was stimulated by the Campbell et al. (2001) poor-grounded claim that CO-CS set leads to significantly better agreement of MC results with experimental data if compared with P&P-CS set.

*Corresponding author.
E-mail address: cenian@imp.gda.pl (A. Cenian).

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2. Model description

Campbell et al. (2001) have proposed MC model based on the isotropic algorithm and the density rescaling procedure proposed by Li et al. (1989) enabling the swarm-parameter determination under high-ionization rate conditions. The use of elastic momentum-transfer cross section in MC simulations enables one to incorporate part of the anisotropy effects (Phelps and Pitchford, 1985a; Cenian et al., 2000) and at the same time, it preserves the simplicity of an isotropic procedure. The transport parameters including Townsend's primary ionization coefficient, drift velocity and the transverse- and longitudinal-diffusion coefficients are determined.

The CO-CS set used by Campbell et al. (2001) is a modified version of the cross sections of Ohmori et al. (1988). The last CS set was compiled from experimental data on the cross sections for elastic, ionization and dissociation processes as well as vibrational (first 10 states) and 20 other inelastic (mainly, electronic state excitation) channels. The data were extrapolated up to 250 eV by Kelly (1990)—some linear scaling techniques were used whenever necessary. The cross sections for the electron impact excitation of the 10 lowest-lying electronic states were later exchanged with the integral cross sections determined using extrapolation procedure (molecular phase shift analyses) of previously measured differential CS (Brunger and Teubner, 1990). The difference between the CS sets (Ohmori et al., 1988; Kelly, 1990; Campbell et al., 2001) is presented in Figs. 1 and 2a (see faint dashed line). The new electronic excitation cross sections produce slight increase of total CS (Fig. 1) in the energy region 10–20 eV.

The standard CS set used by Phelps and Pitchford (1985a) is available on a Internet web site (Phelps and Pitchford, 1985b). The CS set proposed by Kochetov et al. (1979) (KPPS-CS) differs most substantially from P&P-CS set in the dissociation part and in ionization part from CO-CS set.

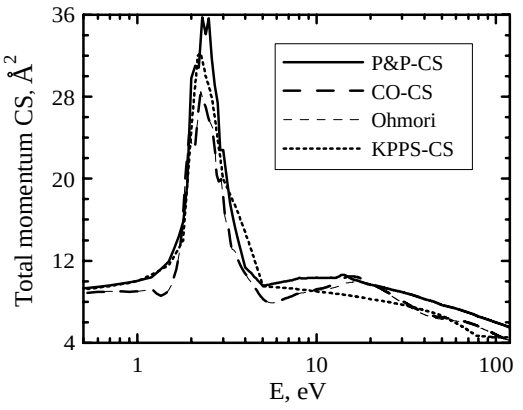

Fig. 1. The total momentum-transfer cross sections: P&P-CS (solid line), KPPS-CS (dotted line), CO-CS (dashed line), and Ohmori et al. (1988) set (faint dashed line).

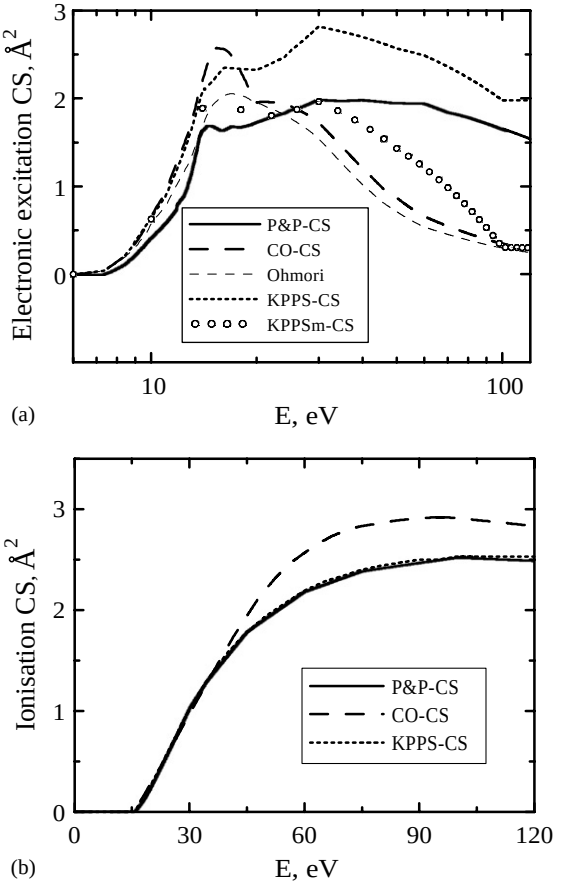

Fig. 2. Cross sections for (a) electronic excitation and (b) ionization: P&P-CS (solid line), CO-CS (dashed line), Ohmori et al. (1988) set (faint dashed line), KPPS-CS (dotted line), and modified KPPSm-CS (open circles).

The dissociation cross sections of KPPS set are close to those given by Cosby (1993). The last CS were not included in the original P&P-CS set, although, they are presented on the Phelps and Pitchford (1985b) www site. It was assumed (P&P-CS set) that the dissociation proceeds via the electronic high-energy singlet-states excitation. Therefore, in Fig 2a, the dissociation CS are presented together with the electronic-states excitation CS. The dissociation CS in the CO-CS set are two orders of magnitude smaller than these of Cosby (1993). This results in much lower values of CO-CS in Fig. 2a. Lately, Kochetov and Dyatko (2002) have revised their KPPS-CS set—they propose to use the implicit dissociation CS (Cosby, 1993) with the scaling factor 0.1 (see open circles in Fig 2a).

The ionization CS of KPPS- and P&P-CS sets are lower than that of CO-CS set (see Fig. 2b).

Eventually, the elastic CS—calculated for KPPS set as a difference between the total CS and the sum of all other CS—become slightly negative in the high-energy region $E > 75\,\text{eV}$ (see Fig. 3a). We have assumed zero for the elastic KPPS-CS in this energy range. The problem of negative values was resolved by adjusting dissociation CS in the latest modification of KPPS-CS as discussed above (Kochetov and Dyatko, 2002).

The vibrational CS, chosen by Phelps and Pitchford (1985b) (see Fig. 3b), are higher in the peak region 1.8–2.7 eV than those of KPPS- and CO-CS sets. The vibrational cross sections do not influence, however, the results at the considered high E/N region, very significantly.

The total CS of both the CO and KPPS sets are lower than the P&P cross sections in the high energy region $E > 5\,\text{eV}$—this will influence drift velocity (see Fig. 5).

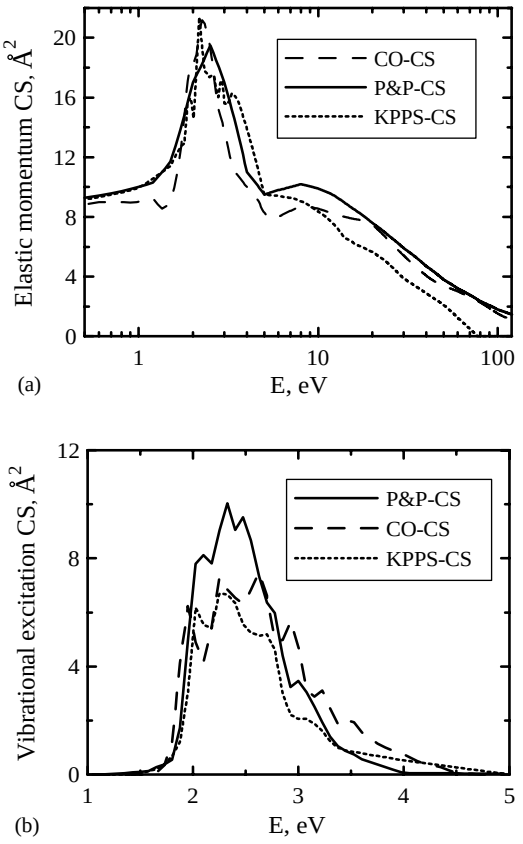

Fig. 3. (a) Elastic momentum-transfer and (b) vibrational-excitation CS: P&P-CS (solid line), KPPS-CS (dotted line), and CO-CS (dashed line).

The presented swarm parameter were calculated applying standard TOF formulas

$$W = \{\langle z(t_2)\rangle - \langle z(t_1)\rangle\}/(t_2 - t_1),$$

$$D_T = \{\langle r(t_2)^2\rangle - \langle r(t_1)^2\rangle\}/4(t_2 - t_1),$$

$$D_L = \{\langle [z_j(t_2) - \langle z(t_2)\rangle]^2\rangle - \langle [z_j(t_1) - \langle z(t_1)\rangle]^2\rangle\}/2(t_2 - t_1),$$

the same or similar to that proposed by Sakai et al. (1977), where

$$\langle X(t_i)\rangle = \sum_{j=1,N_i} X_j(t_i)/N_i$$

and N_i is the number of electrons at time t_i. The direction of electric field is parallel to z-axis. The density rescaling procedure based on introduction of artificial attachment channel (Li et al., 1989) was adopted in order to avoid problems related to electron avalanche at high E/N values. After initial time of equilibration, the trajectories of 200,000 primary (and their secondary) electrons were calculated for the time period, $t_2 - t_1$, equivalent to 1000 or more of real collisions.

3. Results

Figs. 4–6 present the TOF swarm parameters calculated using MC isotropic model described above. As it was already underlined (Cenian et al., 2002), the presented results for CO-CS set agree well, i.e. with

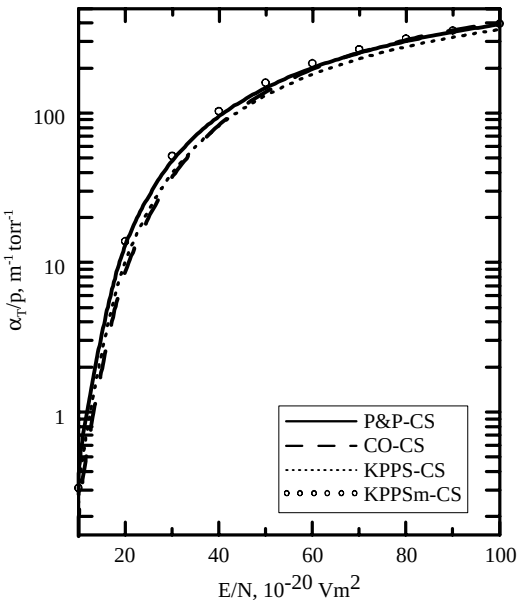

Fig. 4. Townsend's primary ionization coefficient as a function of reduced electric field calculated using various CS sets: P&P-CS (solid line), CO-CS (dashed line), KPPS-CS (dotted line); and modified KPPSm-CS (open circles).

accuracy better than the standard deviation, with the results of Campbell et al. (2001). Furthermore, the agreement of MC results for all considered CS sets with the newest experimental swarm data (Wedding et al., 1985; Kelly, 1990; Roznerski, 1996) is also reasonably good. This confirms the validity of all the considered CS set. It is even more evident, considering the claim of Roznerski (1996) that the differences between his data and of Wedding et al. (1985) "do not exceed the combined errors for the two experiments". The differences between the calculated TOF drift velocities (W) and transverse diffusion coefficients (D_T) for the P&P-, KPPS-, KPPS-mod and CO-CS set are often even smaller than the above-mentioned combined experimental errors.

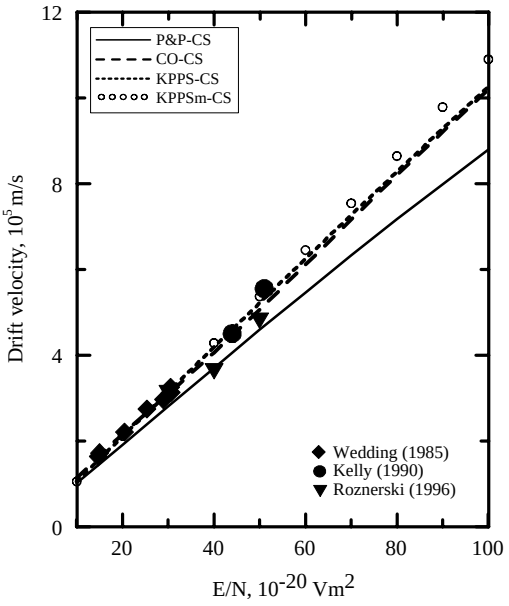

Fig. 5. Drift velocity calculated using P&P-CS (solid line), CO-CS (dashed line), KPPS-CS (dotted line), and modified KPPSm-CS (open circles). Few latest experimental results by Wedding et al. (1985) and Roznerski (1996) are given for comparison.

Fig. 4 confirms, what was already reported by Campbell et al. (2001), that the Townsend's primary ionization coefficients are not very sensitive to the microscopic behaviour in the swarm. One should take into account that ionization CS differs even 20% for P&P- and CO-CS set. Furthermore, it is worth mentioning that the agreement between MC simulation and the experimental data presented in the paper of Campbell et al. (2001) was good—the experimental values were generally slightly above the MC results for CO-CS set. These data are not given in Fig. 4 in order to make figure more readable but they would appear between the results for P&P- and CO-CS sets.

The slightly lower values of drift velocity for the case of P&P-CS set (up to 15% in Fig. 5) is related to the higher values of total CS of this set (electrons loose momentum both in elastic and inelastic collisions). The larger the total CS, the smaller the drift velocities. The total cross sections in KPPS and CO set are close to one another and so the drift velocities. Also, the drift velocities for KPPS-CS set and its modified version (with the total CS being the same) differ less significantly than the respective electron energies and diffusion coefficients—the largest difference is observed for D_L—even up to 20% in Fig. 6b.

The mean (and characteristic) electron energy is mainly effected by the inelastic CS—electrons loose very small amount of energy in elastic collisions. The larger the inelastic CS, the lower the electron energy. Of course, the net result depends on energy threshold for the considered

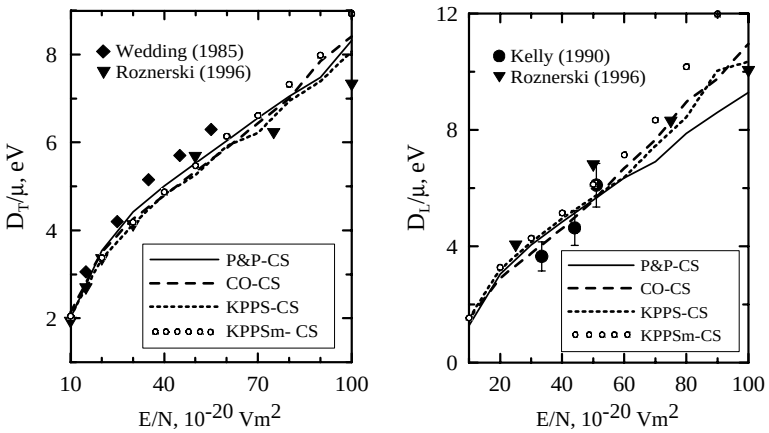

Fig. 6. Diffusion coefficients: (a) transversal (characteristic energy) and (b) longitudinal calculated using P&P-CS (solid line), CO-CS (dashed line), KPPS-CS (dotted line), and modified KPPSm-CS (open circles). Few latest experimental results by Wedding et al. (1985), Kelly (1990) and Roznerski (1996) are given for comparison.

inelastic process. One sees that the characteristic energy (D_T/μ) increases after the reduction of CS for dissociation channel—compare the dotted line (for KPPS-CS set) with open circles (KPPSm-CS set) in Fig. 5.

Furthermore, the total inelastic CS for Campbell and Phelps are not very different in the high-energy range: the ionization CS are higher for CO-CS set but sum of CS for all electronic states excitation is higher for P&P-CS set (mainly due to difference in dissociation and E(sum) CS). Therefore, the characteristic energy does not differ significantly for these CS sets.

The largest differences are found for the longitudinal diffusion coefficient (see D_L/μ in Fig. 6). This should be taken into account when planning new swarm experiments necessary to be completed before the further refinement of CS sets can be continued. Moreover, one should include angular dependence (differential CS) into considerations, as the D_L coefficient is very sensitive to the CS anisotropy.

4. Conclusions

Finally, we conclude that

(1) Basing on the existing experimental data and their statistical errors, it is not possible to make a sound recommendation of the CS set—at least for isotropic approximation. Thus, CO- and KPPS-CS set describe better the characteristic energy measured by Roznerski (1996) but his drift velocities are in better agreement with P&P-CS set. The opposite is true for the measurements by Wedding et al. (1985).
(2) Any further refinement of CS set should be proceeded with new precise experiments, especially of longitudinal diffusion coefficient which is most powerful diagnostic for CS validity.
(3) It is well known that the anisotropy effects increase in the high E/N region, therefore the differential CS should be further investigated and included into high precision calculations.

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