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COMMENT

Comment on 'Integral cross sections for electron impact excitation of electronic states of N_2'

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Abstract

Based on the existing experimental data and their statistical errors, it is not possible to make a sound recommendation of the cross-section set of Campbell *et al* (*J. Phys. B: At. Mol. Opt. Phys.* **34** (2001) 1185). We comment on this paper.

The fundamental importance of molecular nitrogen, both from the theoretical and the practical points of view, has led Campbell *et al* [1] to revisit the problem of determination of electron-scattering cross-sections (CSs) for that molecule. The derived integral CSs for inelastic collisions were incorporated into a set of cross-sections compiled by Ohmori *et al* [2]. An isotropic Monte Carlo (MC) algorithm was applied in order to calculate the transport parameters. Good agreement with measured values was found, in contrast to the striking discrepancy with the high-energy results of Phelps and Pitchford [3]. This is an important issue because the CSs [4] constitute the most popular CS set for nitrogen in use today.

However, the calculations [5] using the Boltzmann equation in the two-term approximation did not confirm the large discrepancy for CS sets [1] and [4]. Further, it was pointed out [5] that the conclusions of Campbell *et al* [1] regarding the usefulness of the cross-section set [4] for electron transport calculations are based on a misleading comparison. The swarm parameters calculated by Phelps and Pitchford [3] for a pulsed Townsend (PT) experiment were related to the experimental [6–8] and the MC simulation [1] results for the time-of-flight (TOF) technique.

Phelps [5] also pointed out that a potentially misleading comparison has been made in [3] by showing the six-term approximation (6TA) results along with TOF experiments in their figure 8, although the associated text does add distinguishing definitions. Already, Sakai *et al* [9] have found that the differences between transport coefficients for various experiments e.g. TOF and PT, can be significant, especially at high E/N.

Our simulations—using an isotropic MC modelling of TOF experiments—confirm the validity of CS set [4]—see the figures. This is even more evident considering the claim of Roznerski [6] that the differences between the results [6] and [7] 'do not exceed the combined

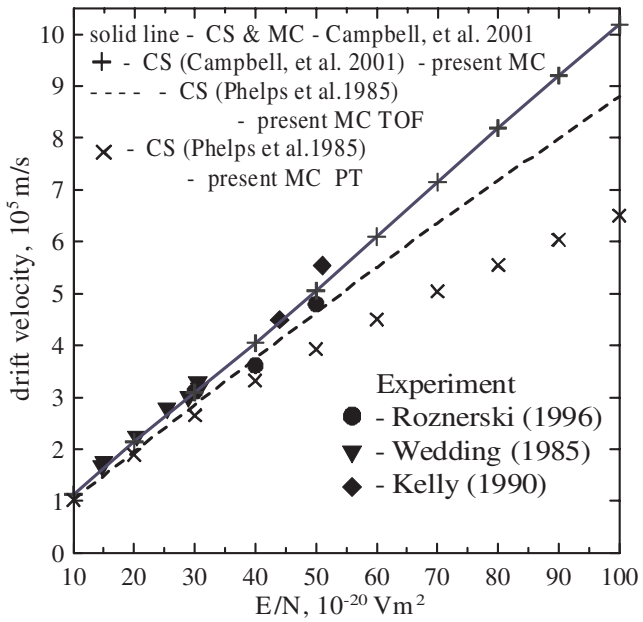

Figure 1. Drift velocity as a function of E/N.

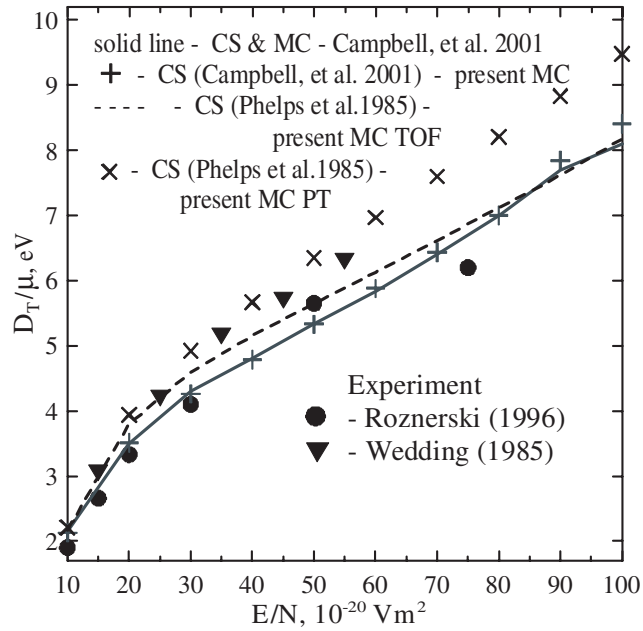

Figure 2. The characteristic energy (D_T/μ) as a function of E/N.

errors for the two experiments'. The differences between the calculated TOF drift velocities (W) and transverse diffusion coefficients (D_T) for the CS sets [1] and [4] are smaller.

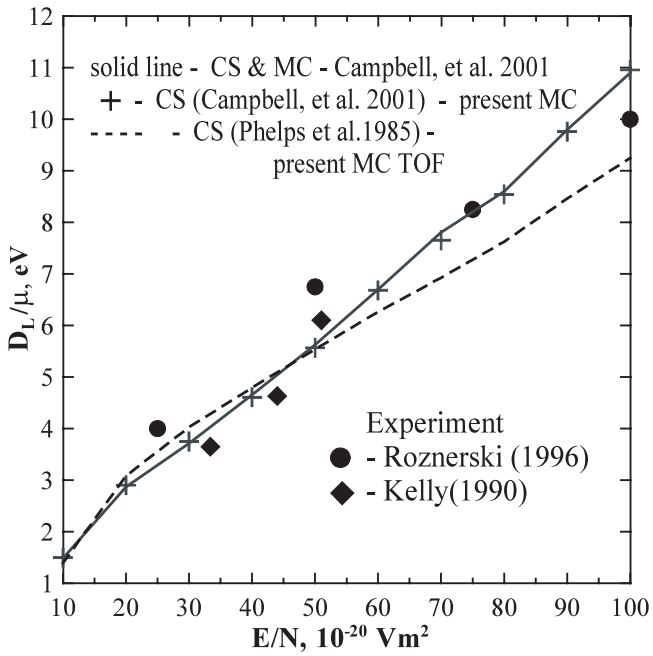

Figure 3. Ratio of longitudinal diffusion coefficient to electron mobility (D_L/μ) as a function of E/N.

The calculations presented here apply standard TOF formulae

$$W = \{\langle z(t_2)\rangle - \langle z(t_1)\rangle\}/(t_2 - t_1),$$
$$D_T = \{\langle r(t_2)^2\rangle - \langle r(t_1)^2\rangle\}/4(t_2 - t_1),$$
$$D_L = \{\langle [z(t_2) - \langle z(t_2)\rangle]^2\rangle - \langle [z(t_1) - \langle z(t_1)\rangle]^2\rangle\}/2(t_2 - t_1)$$

the same as or similar to that in [9], where $\langle X(t_i)\rangle = \Sigma_{j=1,N_i} X_j(t_i)/N_i$ and N_i is the number of electrons at time t_i. The PT formulae

$$W_{PT}(t_i) = \langle v_z(t_i)\rangle \qquad D_{T-PT}(t_i) = \langle [v_x^2(t_i) + v_y^2(t_i)]\theta\rangle/2$$

were taken from [9] for drift velocity and from [10] for the PT characteristic energy (local formula), where v_z is the velocity in the z-axis (electric field) direction and time θ describes the period from t_i to the first real collision. The density rescaling procedure based on introduction of an artificial attachment channel [11] was adopted in order to avoid problems related to electron avalanche at high E/N values. After the initial equilibration time, the trajectories of 200 000 and 500 000 primary (and their secondary) electrons were calculated for the time period t_2–t_1, equivalent to 1000 or more real collisions. This assured that the parameters determined had reached saturated values. The TOF swarm parameters calculated here for CS [1] agree well (i.e. with accuracy better than standard deviation for [1]) with the results of Campbell *et al* [1] based on time derivatives of moments in configuration space.

Finally, we conclude the following.

(1) Based on the existing experimental data and their statistical errors, it is not possible to make a sound recommendation of the CS set [1] or [4]—at least for an isotropic approximation, e.g., thus, CSs [1] describe slightly better the characteristic energy measured by Roznerski [6] but his drift velocities are in better agreement with CSs [4]. The opposite is true for the measurements by Wedding *et al* [7] and Kelly [8].

(2) It is hardly possible to compare two different CS sets based on swarm parameters calculated using different formulae. It was proved that the MC simulation of the TOF experiment gives even 35% higher values for drift velocity (at 1000 Td) than MC results for the PT technique calculated as a space average [9]—see the dashed curve and + in figure 1.
(3) It is well known that the anisotropy effects increase in the high E/N region, therefore the differential CS should be included in high precision calculations (before going to millions of trajectories of electrons).
(4) Any further refinement of a CS set should proceed with new refined experiments or at least thorough analysis of available experimental data in order to choose the most reliable values.

Acknowledgments

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References

[1] Campbell L *et al* 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 1185
[2] Ohmori Y, Shimozuma M and Tagashira H 1988 *J. Phys. D: Appl. Phys.* **21** 724
[3] Phelps A V and Pitchford L C 1985 *Phys. Rev.* A **31** 2932
[4] Phelps A V and Pitchford L C ftp://jila.colorado.edu/collision_data/electronneutral/
[5] Phelps A V 2002 Private communication
[6] Roznerski W 1996 *J. Phys. D: Appl. Phys.* **29** 614
[7] Wedding A B, Blevin H A and Fletcher J 1985 *J. Phys. D: Appl. Phys.* **18** 2361
[8] Kelly L J 1990 *PhD Thesis* Flinders University of South Australia
[9] Sakai Y, Tagashira H and Sakamoto S 1977 *J. Phys. D: Appl. Phys.* **10** 1035
[10] Braglia G L 1981 *Lett. Nuovo Cimento* **31** 183
[11] Li Y M, Pitchford L C and Moratz T J 1989 *Appl. Phys. Lett.* **54** 1403