

COMMENT

Comment on ‘Integral cross sections for electron impact excitation of electronic states of N₂’

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Received 15 July 2002, in final form 1 November 2002

Published 4 December 2002

Online at stacks.iop.org/JPhysB/35/5163

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

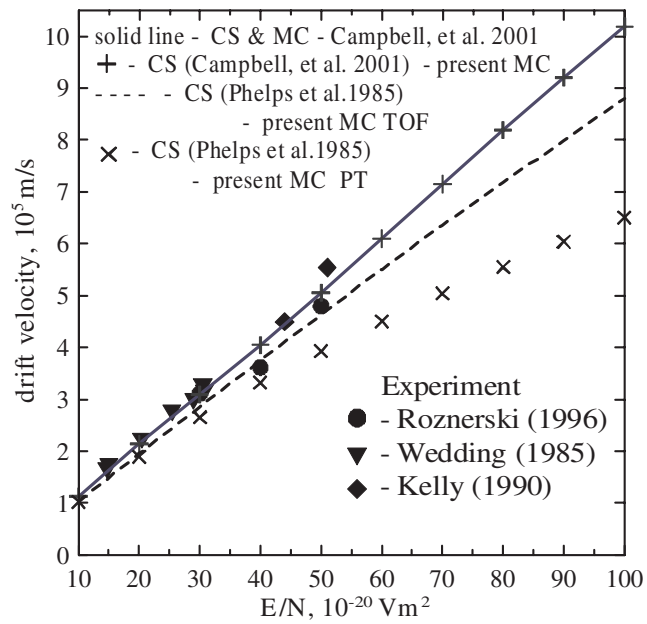


Figure 1. Drift velocity as a function of E/N .

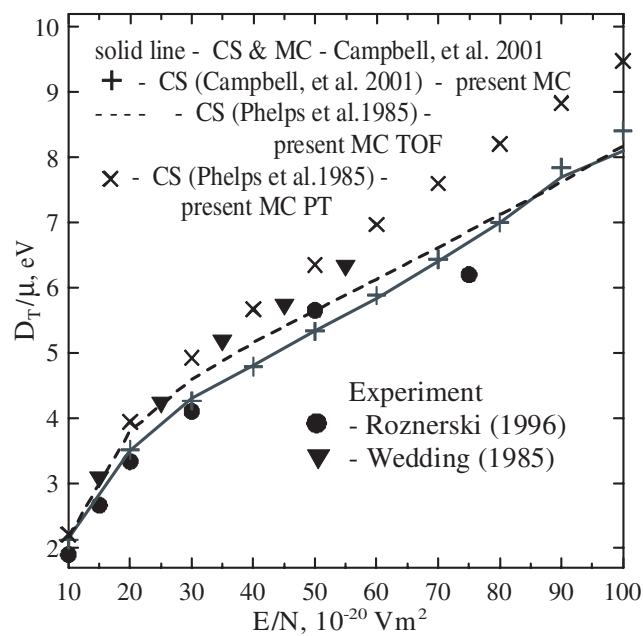


Figure 2. The characteristic energy (D_T/μ) as a function of E/N .

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.

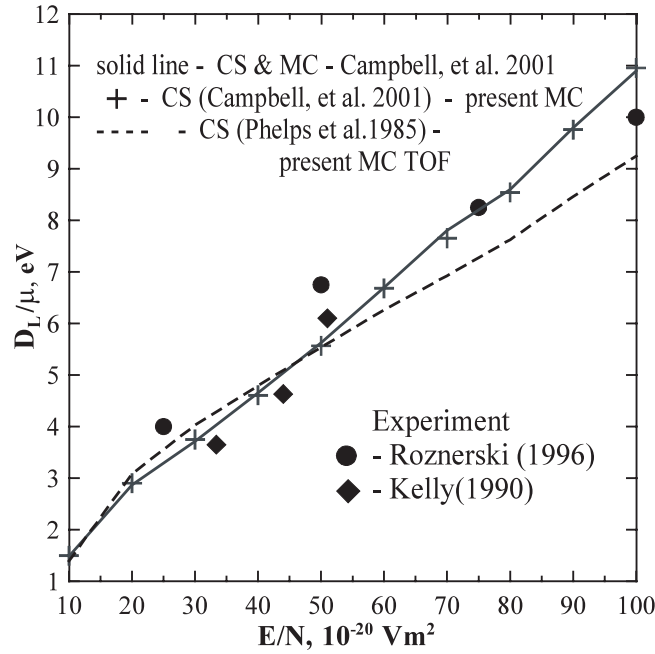


Figure 3. Ratio of longitudinal diffusion coefficient to electron mobility (D_L/μ) as a function of E/N .

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 $\langle X(t_i) \rangle = \sum_{j=1, N_i} X_j(t_i) / N_i$ and N_i is the number of electrons at time t_i . The PT formulae

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

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

The authors acknowledge Dr A M Nolan for sending the CS set [1]. We appreciate the suggestions regarding the directions of this work by A V Phelps.

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