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Monte Carlo simulation of the back-diffusion of electrons in nitrogen

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ABSTRACT

In this paper, the process of back-diffusion in nitrogen is studied by means of Monte Carlo simulations. In particular we analyze the influence of different aspects of back-diffusion in order to simplify the models of plasma displays, low pressure gas breakdown and detectors of high energy particles. The obtained simulation results show that the escape coefficient depends strongly on the reflection coefficient and the initial energy of electrons. It was also found that the back-diffusion range and number of collisions before returning to the cathode in nitrogen are smaller than those in argon for similar conditions.

1. Introduction

Back-diffusion has been the subject of numerous investigations [1–4] due to its relevance for secondary electron emission [5,6], gas breakdown [7,8] and gas-phase multiplication of the charge [9]. Recently, the interest in back-diffusion has been revived in favour of its importance in practical plasma devices [10,11], particle detectors [12,13] studies of breakdown and non-equilibrium effects near the cathode [14,15] and micro-discharges [16,17].

Theoretical studies of the back-diffusion can be broadly divided into two categories. It has either been treated as drift and diffusion of electrons in equilibrium with the applied field or as the beam like collision-controlled back-scattering of electrons near the cathode. The former theories of back-diffusion apply hydrodynamic conditions and coefficients and the latter may be labelled as ballistic (purely non-hydrodynamic) as they rely on analysis of a single or several collisions [18]. The assumption in the latter group of theories is that the return to the cathode occurs after a very small number of collisions with the background gas, most probably only one [19]. The best known theory, represented by the Thomson–Loeb equation has actually become successful only after Loeb modified Thomson's approach, which was purely ballistic, to make a combination of the two assumptions [20]. The third approach was developed recently and it consists of a full, kinetic treatment either by solving the Boltzmann equation or by performing Monte Carlo simulations (MCS) [21,22].

In this paper, results for the escape coefficient, range and mean number of collisions were obtained by using MC code for a wide range of conditions required in modelling. One of the goals of our back-diffusion studies has been to contribute to revision of the application of Townsend's theory to describe the low pressure breakdown [6] which on the other hand may be associated with the ionization and multiplication chambers.

2. Simulation procedure

Monte Carlo simulation (MCS) results presented here were obtained by using the same MC code based on generalized null-collision technique [23,24], as in our previous work on argon [22]. The code allows anisotropic scattering of electrons and takes into account absorbing and reflecting boundaries. It is also possible to define any energy or angular distribution at the boundaries including the numerical experimental data. Calculations were performed by using a well-established set of cross sections that was found to predict accurately the transport in nitrogen [23] and the conditions along the Paschen curve [25]. The primary electrons are treated one by one from their release at the cathode until they reach the anode. When they hit the cathode electron may be absorbed and consequently a new electron is released, or they may be reflected with a given energy loss and angular distribution. The values of the reflection coefficient (number of electrons reflected from the cathode per electron that hits the cathode) were chosen to represent the realistic conditions in the case of poorly reflecting surfaces [26] and in the case of more reflecting metal surfaces [27].

The flux of the initial electrons originated from the cathode varied greatly depending on electric field normalized by the gas

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number density E/N. The number of released electrons was chosen to allow us to determine the coefficients related to back-diffusion with an uncertainty of the order of or less than 3%. Luckily at high values of E/N, the escape coefficient is close to 1 enabling achievement of a good statistics by emitting a relatively small number of electrons. On the other hand, at the lowest E/N we had to release at least 10,000 electrons to attain the required accuracy.

3. Results

The dependence of the escape coefficient f_{es} (defined as the flux of electrons that originated from the cathode and that reach the anode normalized by the initial flux) on the reduced electric field (the electric field to the gas number density) is shown in Fig. 1. As can be noticed from comparison between the simulation and experimental results, MC calculations (solid squares) are in a good agreement with the results of measurements carried out by Wagner and Raether [28] (open squares) and by Hasegawa et al. [29] (open circles).

In Fig. 2(a) we show the effect of the reflection on escape factor for different values of the initial energy and for a fixed E/N. Although, for $R = 1$ f_{es} is 1, for small reflection a limiting value of back-diffusion is reached depending on the E/N and other initial conditions. The fact that coefficient describing the back-diffusion process strongly depends on the initial energy is illustrated in Fig. 2(b). If the initial energy is small the escape factor approaches 1, while if it is large the effect saturates and thus the dependence is non-linear which results in the importance of the definition of the initial energy distribution.

Fig. 3 demonstrates the mean number of collisions as a function of the reduced electric field for three different values of the reflection coefficients of: $R = 0$ (solid squares), $R = 0.24$ (open squares) [26] and $R = 0.6$ (open circles) [27]. The initial electrons are released isotropically from the cathode surface with the energy 1 eV. As in the case of argon, there are no electrons that were absorbed by the cathode after only one collision which is an assumption of many explanations and basic theories. For the reflection coefficients greater than 0, peaks observed for reduced fields between 2 kTd and 3 kTd are due to sharp peaks of cross sections for excitation. These peaks are genuine and considerably larger than the statistical uncertainty of the data which is always less than 3%.

When there is no reflection electrons are rapidly returned to the surface even after a small number of collisions. This is mainly an intrinsic property of the elastic or momentum transfer cross section. Increasing reflection allows electrons to spend more time in the gap. Mean energies for those E/N are 20–50 eV. In other words with no reflection electrons get reflected very quickly and absorbed but if non-zero reflection allows them to return to the gas the number of collisions that they suffer increases as they lose energy in inelastic processes and move to lower energies with very high cross sections. As a result the system has an increased sensi-

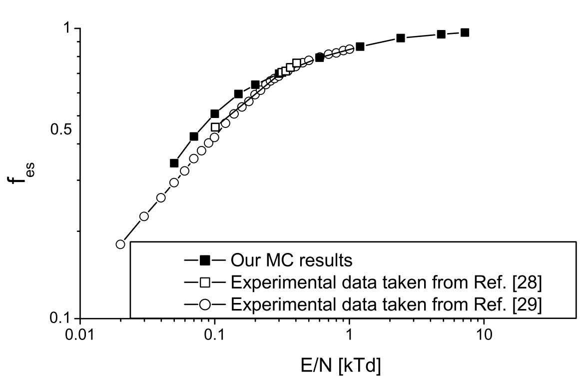

Fig. 1. Escape coefficient as a function of reduced electric field. Results of MC simulations are shown by solid symbols and compared with the experimental data taken from Wagner and Raether [28] (open squares) and Hasegawa et al. [29] (open circles).

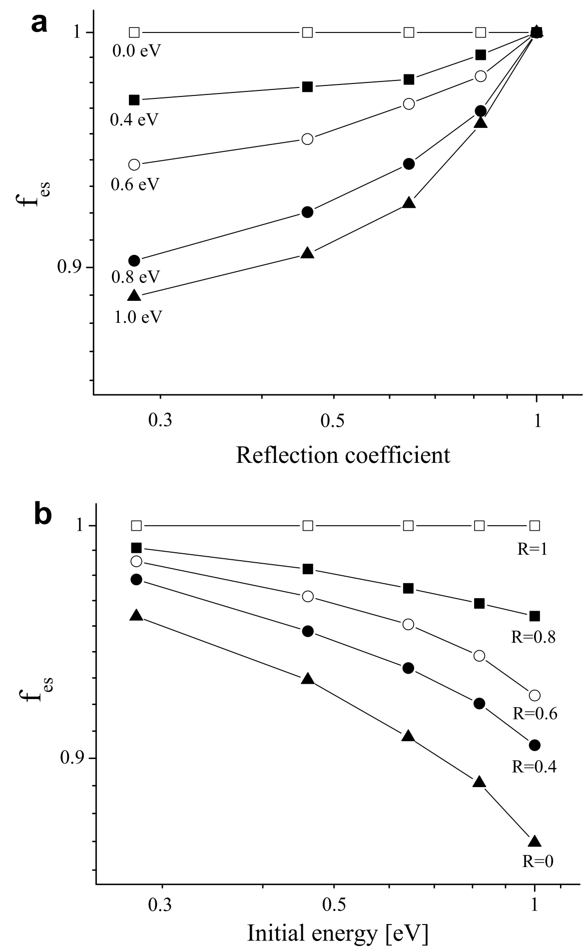

Fig. 2. The dependence of the escape coefficient on: (a) the reflection coefficient for several values of the initial energy and (b) the initial energy for several values of the reflection coefficient. The calculations were performed for a single value of $E/N = 2.4$ kTd.

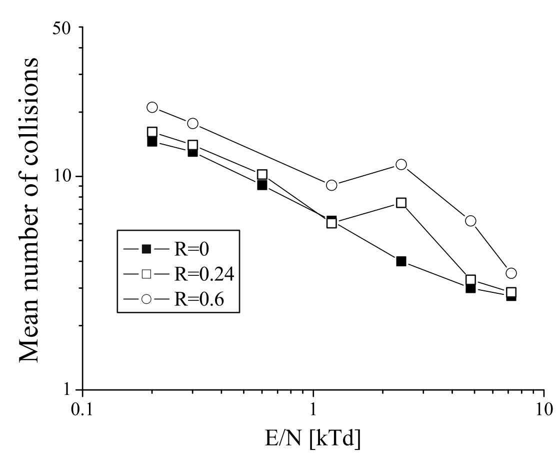

Fig. 3. The mean number of collisions against the reduced electric field for three different values of the reflection coefficient. The initial electrons are emitted isotropically with the energy of 1 eV.

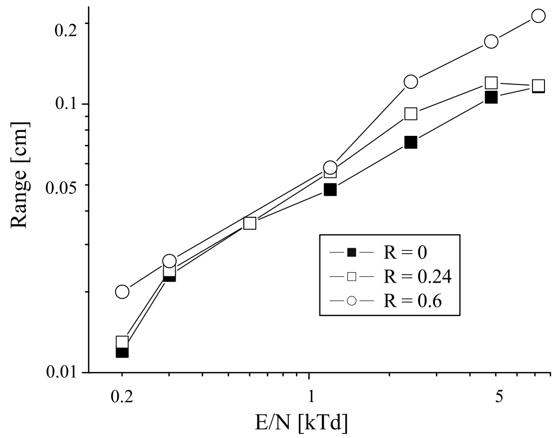

Fig. 4. The range of the electrons depending on the reduced electric field for the reflection coefficient of: $R = 0$ (solid symbols), $R = 0.24$ (open squares) and $R = 0.6$ (open circles).

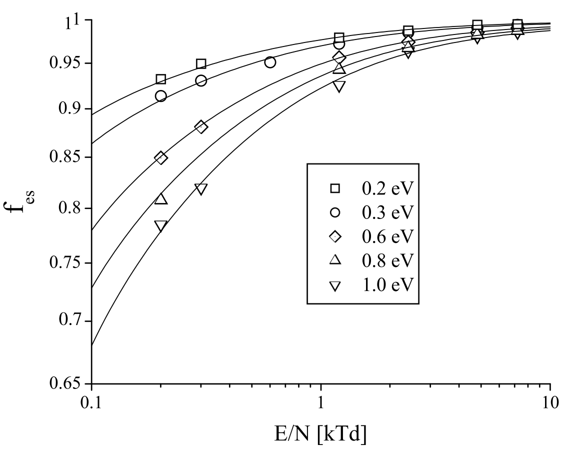

Fig. 5. The escape factor versus the reduced electric field. MC simulation results (symbols) and the corresponding fit (solid lines), for several values of the initial electron energy.

tivity to the reflection in the energy range where a lot of inelastic collisions occur.

As the nature of theory that may be used to describe back-diffusion depends very much on the nature of transport of electrons near the cathode, it is of interest to establish the range of electrons that return to the cathode. In this paper, the range is defined as the maximum distance from the cathode reached by the electron that eventually returns to the cathode. The variation of the range of electrons with the reduced field can be seen from Fig. 4. As expected, the range of electrons is greater when reflection of electrons from the cathode surface is taken into account.

Finally, by choosing appropriate reflection coefficient and/or distribution of the initial electrons excellent fit may be obtained [6]. In Fig. 5 lines correspond to the fit based on the our MC simulation results shown by open symbols.

4. Conclusion

In this paper we have presented and analyzed results concerned with the back-diffusion process in nitrogen. In particular, the influence of the reduce electric field, the reflection coefficient and the initial energy on the escape coefficient were studied. The analysis of our simulation results indicates that reflection has a great effect on the back diffusion at low E/N only if it is large.

The obtained simulation results signify that reflection of electrons will reduce the number of back-diffused electrons and increase the value of the escape coefficient. On the other hand, the effect is much more noticeable at lower values of the reduced filed. It seems that under most conditions covered here number of collisions between emission and absorption at the cathode is quite large and thus after reflection there is a chance that electron will spend significant time in the neighborhood of the cathode and be reabsorbed after repeated collisions with the cathode. It was also found that the initial electron energy distribution is one of the critical parameters and affects the calculated escape factors very much. If the initial energy is small the escape factor approaches 1, while if it is large the effect saturates and thus the dependence is non-linear which results in the importance of the definition of the initial energy distribution. The maximum distance from the cathode was sampled and the distribution of the range of electrons that were absorbed by the cathode was obtained. The obtained simulation results reveal that the range of electrons returning to the cathode exceeds by far mean free path and that the number of collisions that they make before returning is quite large. The conclusions of our investigations allow us to describe the non-equilibrium processes [30,31] close to the cathode with a great accuracy and to include detailed theoretical or experimental data for coefficients participating in the boundary effects.

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