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Back-diffusion of electrons and its process modelling

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Back-diffusion of electrons to the cathode has been analyzed by the Monte Carlo simulation. We have studied the influence of different aspects of back-diffusion modelling in particular, with the primary aim to find out a minimum set of parameters necessary for the simulation of the back-diffusion effect. The results are presented in a form that permits reasonable estimation of the back-diffusion to be expected in experimental situations. The obtained results are useful in modelling plasma displays, low pressure gas breakdown and nuclear particle detectors.

Key words: **back-diffusion, energy distribution, angular distribution, Monte Carlo simulation.**

Introduction

IN this paper we have tried to give a broad view of the back-diffusion process and specify the range of importance of the parameters which affect it. It seems that the primary goal of our researches has been either to produce simplified formulae for application in the plasma modelling or to obtain results that agree with the experimental data. The conclusions of our investigation allow us to describe the non-equilibrium processes close to the cathode with great accuracy and, at the same time, to include detailed theoretical or experimental data for coefficients participating in the boundary effects. Argon has proved to be the most difficult case for investigation. Therefore further studies of back-diffusion are still required.

The process of back-diffusion, due to its relevance for both the cathode and gas phenomena such as secondary electron emission, electron reflection, gas-phase multiplication of charge etc., was a subject of numerous investigations. Recently, the interest in back-diffusion has been renewed, due to its importance in the practical plasma devices such as: plasma display panels, procedure of surface sputtering, switching and lighting, studies of breakdown and non-equilibrium boundary effects near the cathode and in nuclear particle detectors. For example, in nuclear particle detectors, the photoelectron detection in gas media can be reduced, with respect to vacuum, by elastic scattering from the gas molecules and consenquently backscattering of electrons, depending on the gas nature and the reduced field *E/p* (ratio of electric field and pressure of the gas) at the cathode surface. At lower values of the ratio *E/p*, there is a striking evidence of this effect due to the lack of inelastic channels for electron-molecule interactions. At higher *E/p* values, the opening of excitation and ionization channels reduces the backscattering effect and the photoemission yield is close to vacuum values.

Process of back-diffusion

Since the back-diffusion of electrons is a non-equilibrium boundary effect, it plays an important role in the development of gas breakdown and has been studied from the early days of gaseous electronics [1-3]. A series of relatively well defined experiments was performed [4-6] allowing us to improve theoretical and predictive numerical models. Those include the moment theories [7] and the still relatively simple Monte Carlo simulations (MCS) [8-13].

The primary aim of our back-diffusion studies has been to revise the application of Townsend's theory [14] to describe the low pressure breakdown which became apparent from the studies of the volt-amper characteristics of low-current diffuse dicharges and secondary electron yields [10]. It was recently shown that the basic assumption of Townsend's theory [14] that ions produce secondary electrons has an application limited to a small number of cases. The production of initial secondary or feedback electrons is described by the secondary electron yield γ, that can be determined from the gas breakdown data. We were motivated by the fact that the published results for the secondary electron yields from the ion beam experiments and gas discharges are sistematically in a serious disagreement. At the same time, we have tried to bild up a standard procedure for obtaining the secondary electron yield γ. According to the revised Towsend's theory that was suggested by Phelps and Petrović [10] secondary electron production is strongly affected by back-diffusion.

Coefficients describing back-diffusion

Back-diffusion means that electrons, originating from the cathode, collide with the gas molecules above the electrode. A certain number of electrons diffuse back to the cathode and may be absorbed by it, contributing nothing to the current flowing through the gas. The resultant current is, therefore, due to the total charge of electrons given off by the cathode, minus the amount returned to it by back-diffusion. It is obvious that the greater part of the diffusion process is going to occur in the immediate vicinity of the cathode before the electrons have reached thermal and field equilibrium.

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The effect of back-diffusion may be represented by the back diffusion coefficient f_{bd}, which equals the ratio of the flux of back-diffused electrons normalized by the initial flux, or the electron escape coefficient f_{es}, equal to the flux of electrons that originate from the cathode and reach the anode normalized by the initial flux.

The relationship between the two coefficients is simple

$$f_{bd} = 1 - f_{es} \tag{1}$$

The back-diffusion determines the secondary electrons production, so that the effective secondary electron yield γ_{eff} depends on the escape factor f_{es}

$$\gamma_{eff} = \gamma f_{es} \tag{2}$$

Determination of the escape coefficient f_{es}

Determination of coefficients attributed to back-difusion has changed significantly in the recent years. Detailed historic reviews of various aspects of back-diffusion comprising both data on the pioneering works [1-3] and the latest investigations [10-13,15] have already been given. For that reason we shall not atempt to give such a review here, except for remarks about the papers with direct impact on the topic discussed here.

The theoretical studies of back-diffusion process can be broadly divided into two categories. The problem has either been treated as electron drift and diffusion of electrons in equilibrium with the applied field or as the collision-controlled back-scattering of electrons near the cathode where electrons retain their energy of ejection ε_0.

The second category of studies originate from the single collision theory of Young and Bradbury [2] based on the assumption that the constant electron mean free path λ is determined by the initial energy of electrons ε_0.

The most famous formula for determining the escape coefficient is the Thomson-Loeb formula [1]

$$f_{es} = \frac{1}{1 + \frac{v_0}{4v_d}} \tag{3}$$

where v_0 is the initial velocity of electrons emitted from the cathode and v_d is the drift velocity of electrons. We have to mention that eq.(3) was developed by Thomson, while Loeb has put it into a suitable, well-known verification form [1,2].

To calculate the escape factor f_{es} in the geometry of two parallel plate electrodes, Langmuir [2] proposes an equation in the following form

$$f_{es} = \frac{4}{3}\frac{\lambda_e}{d}\frac{V}{\varepsilon_0}\frac{1}{\log\left(\frac{V}{V+\varepsilon_0}\right)} \tag{4}$$

in which V is the potential across the plates, d is the gap between the plates, ε_0 is the energy ejecting the electrons from the cathode and λ_e is the mean free path of the electron in the gas. The base for deriving relation (4) is the well-known diffusion equation of electrons in an electric field suggested by Hertz [2]. Essentially, the derivation applies the same principles as the Thomson equation, i.e., it considers the number of electrons lost from the initial saturation current by diffusion back to the emitting electrode.

The experimental studies were initiated by Thomson [1]. Brabury [2] measured the back-scattered photoelectrons ejected from a plane cathode with the initial electron energy of 0.8 eV. Theobald [4] first established for a variety of gases and values of the product pd>100 Torrcm (p is pressure and d is the interelectrode separation) that the escape coefficient depends on the reduced field E/p only and not on p or d separately. Dahlquist [5], with a view to obtaining a fine control over the initial energy ε_0, measured the escape fraction f_{es} for thermionically emitted electrons in argon, transmitted through a mesh cathode for the values of ε_0 between 2 eV and 3.5 eV. The comparison of our results with the experimental data of Thobald [4] and Dahlquist [5] is given next. Felsch and Pech [6] measured the escape coefficient in argon for the values of ε_0 between 0.33 eV and 0.9 eV.

In their experiments, high values of reduced field E/p were applied without the occurrence of ionization. It was done by single-electron collisions in the gas, by keeping the voltage applied across the electrodes beneath the gas ionization potential. Bekarian and co-workers [7], who have performed measurements of the back-diffusion of photo-electrons in a system of cylindrical geometry, pointed out the necessity of allowing for the reflection of electrons, which, moving against the applied field, are incident to the cathode.

Lastly, Burch and Whealton [15] have performed a Monte Carlo calculation, with the assumption that the mean free path of electron is constant, which confirms the validity of the Thomson-Loeb formula (3). What they have found out is that an electron will undergo a number of collisions before being absorbed. For electrons which still had the same ratio of emission speed to drift speed v_0 / v_d after reflection, the following equation can be derived

$$1 - f_{es} = \frac{(1-(f_{es})_0)(1-R)}{1-(1-(f_{es})_0)R} \tag{5}$$

where $(f_{es})_0$ is the escape coefficient without reflection i.e. at R=0, f_{es} is the escape coefficient corresponding to the reflection coefficient R.

In the paper of Vidau and von Engel [7] the effect of back-diffusion has been reanalysed in terms of one-dimensional diffusion and drift with allowance made for the Ramsauer-Townsend effect, which causes the electron energy and mean free path to vary from its initial value at the cathode to its equilibrium value. By solving the equation for electron transport for the plane geometry, neglecting the electron attachment, excitation, ionization and space-charge effect, Vidaud and von Engel [7] have obtained analytically the expression for the ratio of collected to emitted current densities that corresponds to the escape coefficient f_{es}

$$f_{es} = \{1 + 3.14\varepsilon_0^{1/2}(1-R)\left[3.16(E/p)^{1/4} + \varepsilon_0\right] - \\ -(1-R)\varepsilon_0^{1/2}\left[\frac{0.53}{(E/p)^{1/8}} + \frac{21.1}{(E/p)^{1/2}}\right]e^{-0.316(E/p)^{3/4}pd}\}^{-1} \tag{6}$$

where is the initial energy of electrons, E is the electric field, p is the pressure of the gas and d is the electrode separation. Eq.(6) predicts that for a given ratio E/p and the itial en

trons have not reached their equilibrium energy before arriving at the anode.

Di Mauro and co-workers [8] have also treated the problem of back-diffusion using the Monte Carlo simulation. They have performed calculations and experimental measurements for argon, methan and different gas mixtures, bearing in mind the application of their results in nuclear particle detectors. In their Monte Carlo code the input parameters were the components of gas mixtures, electric field, pressure and temperature of the gas as well as maximum electron energy. In their calculations, they have used the Gaussian initial distribution with the mean energy of 0.26 eV. The agreement between the simulations and experimental results is statisfactory and the behaviour of different gas mixtures is fairly well reproduced. Consequently, they have attributed a major part of the photoelectron collection efficiency reduction observed in the investigated gas mixtures, to the backs-cattering phenomenon, the only one considered in their simplified model of electron transport.

The fractional energy transfer in an elastic collision is given by the relation:

$$\frac{\Delta\varepsilon}{\varepsilon} = \frac{2mM}{(m+M)^2}(1-\cos\theta) \tag{7}$$

where m and M are respectively the electron and gas molecule masses and ϑ is the scattering angle in respect to the electron trajectory just before the impact. Due to the large mass difference, the energy loss per collision is very small, resulting in a wide range of scattering angles and in a high probability that some photoelectrons, backs-cattered towards the photocathode, will not be detected. In elastic collisions, the electron direction of motion is only slightly perturbed. Therefore, in the framework of their simple model [8], the photoelectron collection efficiency is determined primarily by the ratio of elastic and inelastic collisions: the rate of inelastic collisions is large, while the backs-cattering probability is very small. It has been confirmed that the photoelectron collection efficiency in the gas media can be reduced, with respect to vacuum, by the elastic backs-cattering from the gas molecules, depending on the gas nature and the ratio of the electric field and pressure *(E/p)* at the cathode surface. However, Di Mauro did not perform a systematic analysis of the back-diffusion process as a function of different parameters (as it was done in this article) and our conclusions are complementary to the results of Di Mauro and co-workers [8].

Phelps and Petrović [10] have given a semi-empirical expression for the escape fraction f_{es}

$$f_{es} = \left(1+\frac{\left[(\varepsilon_0/0.6)^2+(E/N)^2/30\right]}{\left[1+(E/N)/30\right]}\frac{100}{(E/N)}\right)^{-1/2} \tag{8}$$

where the E/N value (electric field normalized by the gas number density) is in *Td* ($1Td = 10^{-21}$ Vm^2) and ε_0 is the energy of the electrons ejected from the surface in eV. For the initial energy of 0.6 eV the second exponent in eq.(8) should be reduced to about *1* so eq.(8) gets a simplified form

$$f_{es} = \frac{1}{(1+100N/E)^{1/2}} \tag{9}$$

Recent theoretical results by Nagorny and Drallosa [9] are barely distinguishable from the empirical fit (8). However we have to note that eq.(8) is only a semi-empirical fit and depends on the initial energy, so it is valid in a reduced range.

Monte Carlo simulation

The calculations of back-diffusion and escape coefficients were performed using a Monte Carlo code and a complete set of electron scattering cross sections that accurately represent collisions in argon [16,17]. The utilized Monte Carlo simulation code is based on the generalized null-collision technique. The set of cross sections that was used involves 27 inelastic (excitation) processes, ionization treated as non-conservative process and elastic scattering. Each of these processes has associated differential cross sections which are only necessary for establishing the angle of scattering. The probability of scattering i.e. the free path is determined on the basis of the total cross section. We have made sure that the corresponding momentum transfer cross section is in good agreement with the standard momentum transfer cross section for argon.

Monte Carlo code

General characteristics of our Monte Carlo code include using Knuth's random number generator *ran3* [18]. The random number generator *ran3* is taken from the second edition of *Numerical recipes* [18] and it is the only random number generator which has not been changed from the first edition. Unlike a great number of random number generators which are based on linear congruental method, the random number generator *ran3* is based on the subtractive method.

At the moment of collision, the decision about whether the real or null collision occurs is made by using one random number. The same number is used to establish which of the possible real collisions take place, based on collisional frequencies. The scattering angle of electrons is determined by another random number.

The time of the next collision is determined from the total collision cross section (frequency) so the differential cross sections are used simply for determining the direction of the scattered electrons, i.e. they are normalized to the total cross section. The momentum cross section is also calculated from the total cross section and the angular dependence of scattering and is compared with the swarm data.

The 'anisotropic' collisional processes are assigned the effective differential cross sections in as large a number of energy regions as was found necessary to describe the process properly and have smooth transitions. The scattering angle ϑ of the incoming electron after the collision event was calculated from the random number ξ by

$$\xi(\vartheta,\varepsilon) = \frac{\int_0^{\vartheta}\sigma_k(\vartheta,\varepsilon)\sin\vartheta d\vartheta}{\int_0^{\pi}\sigma_k(\vartheta,\varepsilon)\sin\vartheta d\vartheta} \tag{10}$$

where ε is the incident electron energy.

The recoil energy transfer from the incoming electron to the heavy molecular particles in elastic collisions has been taken into account once the scattering angles have been determined.

The code testing

The code has been developed and tested in the Institute of Physics and has proved to give the accurate electron en-

ergy distribution functions and transport coefficients in model gases and in argon [17]. Both isotropic and anisotropic model of Reid were used [17,19,20]. In all the cases, the agreement was statisfactory.

Simulation conditions

Back-diffusion is a non-equilibrium effect that is difficult to include in the Boltzman equation analyses of discharges [9]. It was shown that the Monte Carlo simulation is an ideal technique for studying the influence of different parameters (initial energy, energy distribution function, reflection of electrons, energy loss in collisions with surface, etc.) on the back-diffusion.

The Monte Carlo code that was used in this paper has been developed to survey electron transport in parallel plate geometries with complex boundary effects. We have added, to the already existing code, a part that checks if electron goes back to the cathode after collision or continues travelling to the anode. Furthermore, we have considered the reflection of electrons from the cathode, bearing in mind that electrons are reflected from the cathode surface without any energy loss. In other words, the code follows individual electrons released from the cathode until they reach either anode or cathode. When an electron hits the cathode it may be absorbed, causing a new electron release, or it may be reflected with the given energy and angular distribution.

The electrons we have released from the cathode with initial flux varied greatly, depending on the electric field normalized by the gas number density *E/N* and on *N*. Luckily, at high *E/N* where the back-diffusion coefficient is quite small, the number of collisions as electrons cross the gap is also small, so it was easier to achieve good statistics by releasing a relatively small number of electrons. At the lowest *E/N* the number of starting electrons to achieve the required accuracy is 10,000.

Electron initial energy has also been altered. In order to compare our results with the available experimental data, electrons with the initial energy of 0.3 eV and 0.6 eV, or 0.2 eV were emitted to obtain results using the Thomson-Loeb formula [13]. However, in most cases it is presumed that the electrons originate from the cathode, their initial energy being 1 eV.

The maximum distance from the cathode was sampled and the distribution of the range of electrons that were absorbed by the cathode obtained. Furthermore, we have recordered the number of collisions before each electron was absorbed by the cathode. The standard position of the anode was at 1 cm from the cathode, but it was often assumed to be closer, to speed up the simulation. It was done by allowing the distance to be at least five times longer than the maximum range that was detected in the trial run. The reflection coefficient was elected to represent the realistic conditions i.e. metal cathode. The number of emitted electrons was chosen to allow us to determine the coefficients related to the back-diffusion with an uncertainty of the order or less than 2%.

Bearing in mind the application of the obtained results in breakdown modelling, calculations were performed for the *Paschen* curve exact conditions, as cited in reference [10]. Under those conditions pressures for very low values of reduced field *E/N* become very high and a huge number of collisions are required to model the data. Thus we could not extend those data below 9 *Td* for the actual conditions of the *Paschen* curve. To illustrate this, we will mention that for the reduced field of 9 *Td* and the initial number of 10,000 electrons, the calculations last for more than ten days.

The described Monte Carlo code helped us to study the influence of different aspects of back-diffusion modelling. It was concluded that the initial electron energy distribution is one of the critical parameters and affects the calculated escape factors, to a great extent. The same is true for reflection while the angular distribution of initial electrons has a very small influence on the escape factor. Most importantly, it was found that the range of electrons returning to the cathode exceeds the mean free path by far and that the number of collisions that they make before returning is quite large.

Before we started the calculations the code was tested, one of the important tests being to release electrons with zero energy. As expected, in all the cases we have obtained, the escape coefficient $f_{es} = 1$. When electrons start with zero energy thay can not reach the cathode as they are scattered back due to a very small loss of energy in elastic collisions [21].

Results

The escape coefficient f_{es} was calculated for a wide range of conditions required in modeling. The influence of the reflection coefficient was analysed in particular, then the influence of the initial energy and the initial energy distribution function and finally the influence of the angular distribution on the escape coefficient. In all those studies the real data for the standard model [11-13,17,21] was used and compared it with calculations, one of the properties described by a simplified model.

Semi-empirical and the Thomson-Loeb formula

Fig. 1 shows the basic data obtained by the Monte Carlo simulation and compares it to the analytic formula given by Phelps and Petrović [10]. The agreement between predictions of the semi-empirical formula, eq.(8) (for the initial energy of 0.3 eV) i.e. formula eq.(9) (for the initial energy of 0.6 eV) and the Monte Carlo simulation results is quite good, though the Monte Carlo simulation results are systematically lower. However, by choosing the appropriate reflection coefficient and initial electrons distribution, an excellent fit may be obtained.

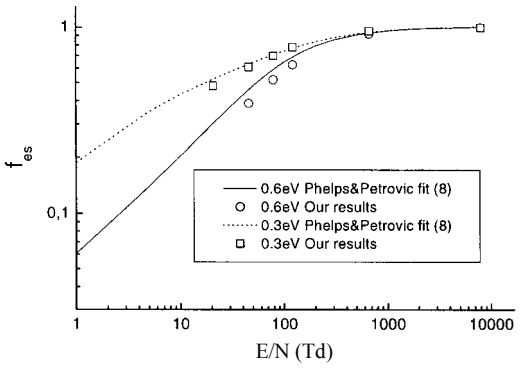

Figure 1. Comparison of the Monte Carlo simulation results (symbols) with the semi-empirical formula of Phelps and Petrović [10] (curves), for two different initial energies, the reflection coefficient R=0.6 and the isotropic angular distribution of initial electrons

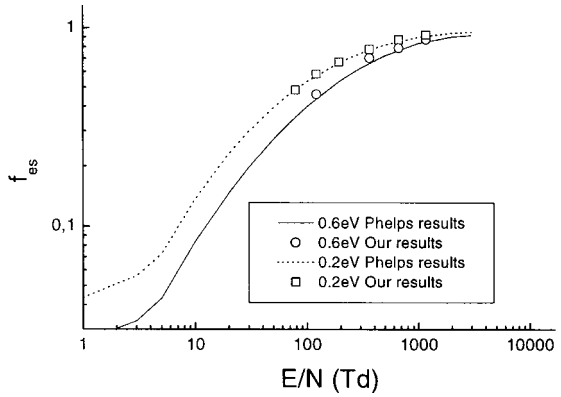

Figure 2. Dependence of the escape factor f_{es} on the reduced field. The results were calculated using the Thomson-Loeb formula, eq.(3) (R=0.6 and initial electrons are isotropically released from the cathode)

Fig.2 presents the escape coefficient f_{es}, acquired by the Thomson-Loeb formula, eq.(3) for two different initial electron energies of 0.2 eV and 0.6 eV. Our results (symbols) were compared with the appropriate Phelps results (curves).

The influence of the initial energy and the reflection coefficient

One of very important parameters that has to be included in the analysis of the back-diffusion is the reflection of

von Engel (6) are shown. The effect of reflection may be estimated from a simple formula based on a single collision model of the back-diffusion

$$f_{bd}(R) = f_{bd}(0)\frac{(1-R)}{1-f_{bd}(0)R} \qquad (11)$$

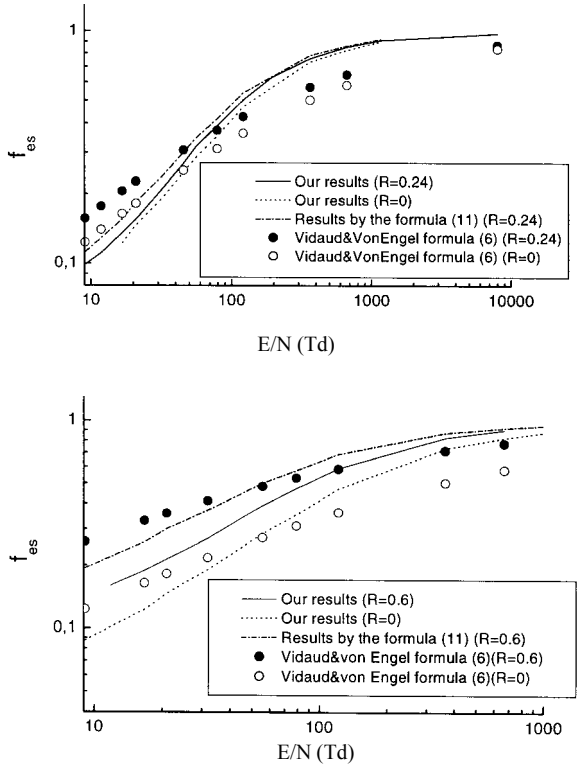

Figure 6. The effect of the reflection on the escape factor. The results are obtained for two values of the reflection coefficient a) R=0.24 and b) R=0.6, the initial energy of electrons 1 eV and the isotropic angular distribution.

The application of eq.(11) overestimates the effect of reflection. It seems that, under most conditions covered here, the number of collisions between emission and absorption at the cathode is quite large. Thus, there is a chance that after reflection an electron will spend a significant time in the vicinity of the cathode and be absorbed after repeted collisions with it. This is much better observed in Fig.6b, for higher values of the reflection coefficient. The formula of Vidaud and von Engel (6) for both values of the coefficient R, has a different shape but the same order of the reflection effect as that predicted by eq.(11).

It can be concluded that the back-diffusion is significantly influenced by large reflections. However, in practice, we have values halfway between the predictions given by eq. (11) and calculations disregarding the reflection effect (R=0).

The effect of energy and angular distribution of initial electrons

To compare the results of our simulation with those of the Monte Carlo simulation acquired by Di Mauro and coworkers [8], we have performed calculations in case of electrons released from the cathode surface with the Gaussian initial energy distribution, the average energy being 0.26 eV. The obtained results and their comparison with the results of Di Mauro [8] are shown in Fig.7.

Fig.7 shows that a difference between the results of our simulations and the results of Di Mauro exists even for a field reduced by a few *Td-s*. It must be mentioned that the results of Di Mauro and co-workers [8] for argon are not similar to the experimental data. Taking into account that the agreement of our results with the appropriate experimental data is excellent (Fig.13 and 14) we may conclude that Di Mauro has made an error in the numerical procedure.

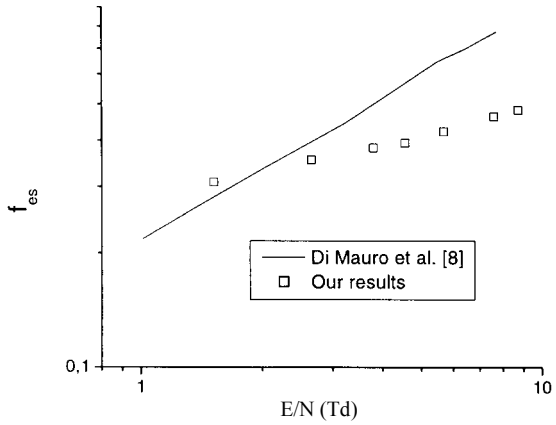

Figure 7. The influence of the initial energy distribution function on the back-diffusion for a Gaussian initial distribution (curve) with the mean energy of 0.26 eV. The results of Di Mauro [8] are presented by symbols. (The gap between the electrodes is 1 cm, the reflection coefficient is R=0.6 and electrons are released isotropically)

The comparison of the back-diffusion coefficients for two different initial distributions: monoenergetic and Maxwellian, both with the same mean energy, is shown in Fig. 8b. Both distributions are real, the first one in photoemission and the second one in electrons behaviour modelling.

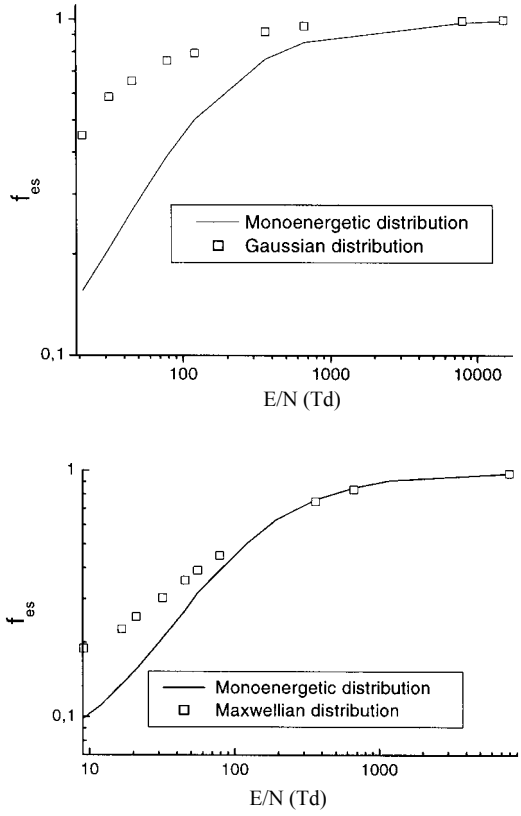

Figure 8. The effect of the initial energy distribution function on the back-diffusion for the monoenergetic (curve) initial distribution with the distribution function: a) Gaussian with the mean energy of 0.26 eV (symbols) and b) Maxwellian with the mean energy of 0.6 eV (symbols) (R=0.6, d=1 cm and the isotropic angular distribution)

It is evident from Fig.8a and 8b that at higher *E/N*, the back-diffusion efect is the same in both cases. The difference is observable at lower *E/N* and, as expected, with the Gaussian or Maxwellian initial distribution, a considerably larger escape coefficient is obtained. Since the escape factor f_{es} dependence on the initial electron energy is strongly non-linear, the electrons with the initial energy lower than the mean energy have a far greater chance to reach the anode than both the mean energy and high energy electrons. Thus either the Gaussian or Maxwellian distribution gives considerably large f_{es}.

The angular distribution of electrons is another important characteristic of the electrons emitted from the cathode. In Fig.9 we show the results calculated for a monoenergetic group of electrons of the same energy released either isotropically or along the axis of the electric field (in this case along the *z* axis). The difference is very small but the z-directed electrons have a greater chance to reach the anode.

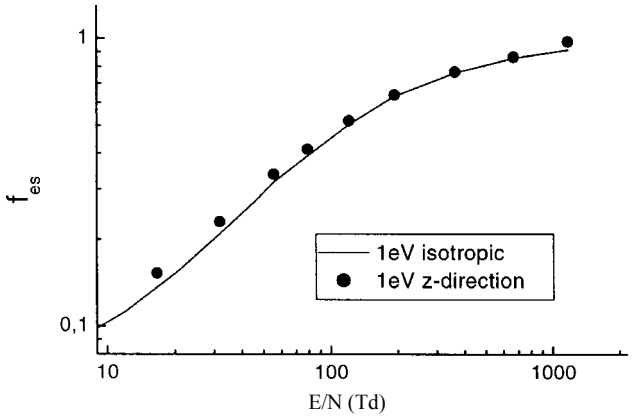

Figure 9. The dependence of the escape factor on the initial angular distribution of the electrons. The isotropic angular distribution of the inital electrons is presented as a solid line and the initial distribution perpendicular to the cathode by symbols. The calculations were performed for the initial energy of 1 eV, the reflection coefficient of 0.6 and the distance between the electrodes of 1 cm

The isotropically emitted electrons have a smaller component of velocity along the *z* axis. However, since the number of collisions is quite large so is their chance to be diverted in the direction of the field and reach the anode.

Spatial range and the mean number of collisions of the back-diffused electrons

The nature of theories that may be used to describe the back-diffusion depends significantly on the nature of transport of electrons that the cathode may absorb. For that reason it is important to establish the range of electrons that return to the cathode. We define *range* as the maximum distance from the cathode reached by an electron that eventually returns to the cathode. In other words, electrons that go beyond the maximum range have no chance of returning.

The distribution of ranges for the same value of the reduced field *E/N*=12 *Td* and for three different pressures are shown in Fig.10.

Simultaneously, the mean number of collisions for the same conditions was being determined. To our surprise, it was found that no electrons were absorbed by the cathode after only one collision, which is at the root of numerous explanations and basic theories. The mean values of the collision number at a fixed *E/N* as a function of of pressure are presented in Fig.11a. It may be observed that the mean number of collisions before the re-absorbtion is quite large and the range is significantly larger than the mean free path, for e.g. for the pressure of 0.5 *Torr,* the range is around 1 cm. This statement is in accordance with the theory of Nagorny and Drallos [9].

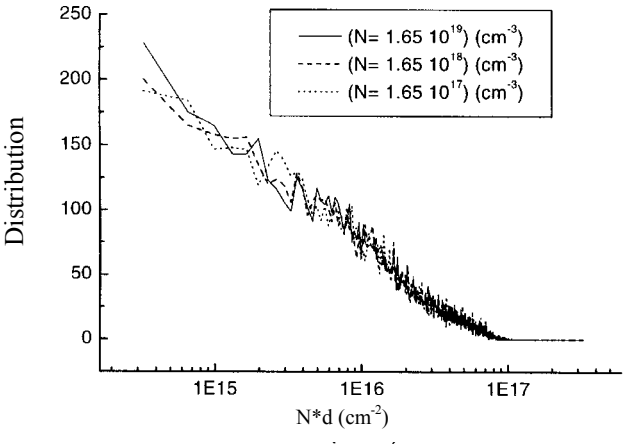

Figure 10. The distribution (the number of electrons that have reached a certain distance) of the largest distance from the cathode (ranges) reached by the back-diffused electrons. The results were obtained for 10,000 initial electrons isotropically released from the cathode, with the initial energy of 1 eV and the reflection coefficient of 0.6

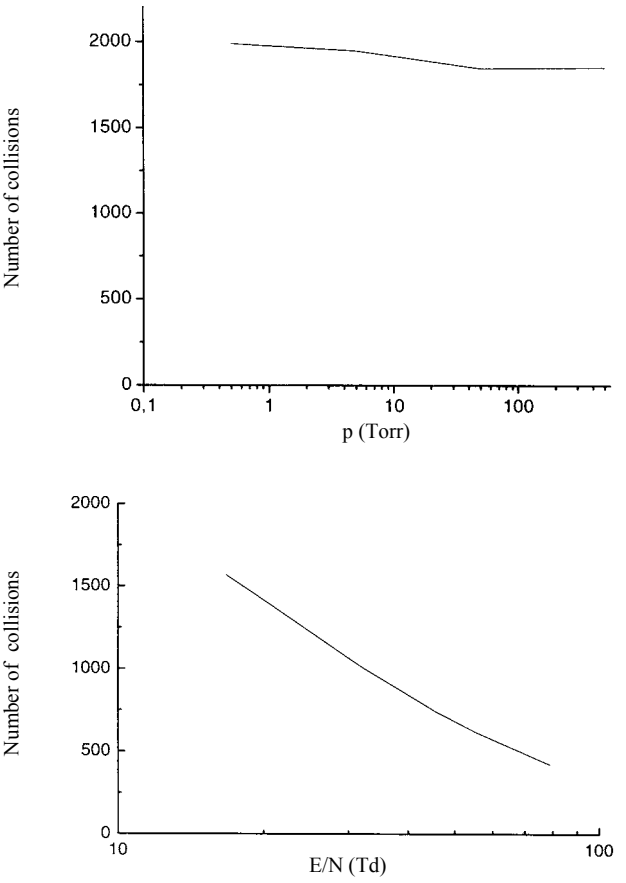

Figure 11. The mean number of collisions as a function of : a) pressure (equivalent to gas number density *N* at 293 K) for the fixed *E/N*=12 *Td* and b) the reduced field *E/N*. The results correspond to the initial energy of electrons ε_0=1 eV, the reflection coefficient *R*=0.6 and the isotropic angular distribution

The range profiles scale very well with the pressure, i.e. the range scale with *pd* (the pressure is denoted by *p*, the

gap between the electrodes is denoted by d). Consenquently, the mean number of collisions depends very slightly on the pressure, while the dependance on the reduced field is strong, decreasing as the reduced field increases (Fig.11b).

One should also bear in mind that the range of electrons that are diffused back to the cathode overlaps strongly with the non-equilibrium or non-hydrodynamic region of the gas discharge and thus one may not expect the equilibirum transport coefficients to be applicable.

The dependence of the range on the pressure being linear, one may suppose that in case of low pressure the range would overlap with the anode and the pressure would depend on the back-diffusion. Another form of pressure dependedence was discussed by Smejtek and co-workers [24]. It is due to high pressure effects on the electron transport; no pressure dependence was found for argon with gas number densities up to $3\times10^{21}\,\mathrm{cm}^{-3}$. It is very interesting to note that both the low and the high pressure effects reduce the back-diffusion.

Pressure dependence

From Fig.12 the escape factor f_{es}-pressure dependence can be seen. The dependence is not present until the pressure becomes low enough to allow the overlaping of the back-diffused electron range with the anode which occurs at a suprisingly large gas number density of $10\times10^{16}\,\mathrm{cm}^{-3}$. The difference between the results acquired for the lenght of the gap exceeding 20 cm and that obtained at 1 cm at low pressures indicates that, for lower densities the escape factor will become pressure-geometry dependent and the transition occurs at the pressure of around 3 *Torr* for the given reduced field of 12 *Td*.

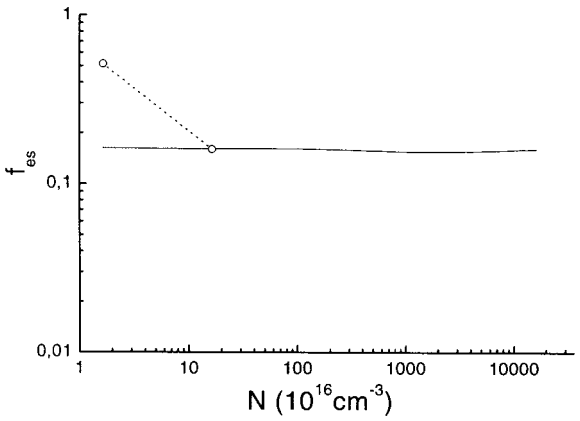

Figure 12. The dependence of the escape factor on the gas number density i.e. pressure. The solid line represents the calculations performed for the gap between the electrodes several times greater than the maximum range of the back-diffused electrons. The symbols represent calculations for the

Should we model the data of Dahlquist [5] that was obtained by the photo emission technique in a fashion similar to that of Theobald [4], by using the monoenergetic initial conditions, an excellent agreement is achieved (see Fig. 14). However, for the data of Dahlquist with the electron mean energy of 1.4 eV, it is not necessary to use the initial distribution different from the monoenergetic beam to achieve good agreement.

Conclusion

Phelps and Petrović [10] have performed a detailed analysis of the breakdown in argon, proving that the production of secondary electrons at the cathode surface is mostly initiated by photons and not by ions hitting the surface. The requirement to model the breakdown included the calculation of the back-diffusion coefficients. In that sense, they have developed a semi-empirical fit (8) which covers a wide range of conditions and situations. There are several measurements of effective electron transmission to the bulk of discharge, but there are few theoretical papers or simulations available in the literature.

Ever since the work of Di Mauro and co-workers [8], the Monte Carlo simulations have been used to study the boundary effect close to the metal electrodes [10-13,21]. In this paper a detailed model of argon, including the cross sections for differential scattering of each inelastic process numerous energies and for the elastic scattering was used to explain the most important aspects of electron back-diffusion modelling. We analyse the influence of different parametres (the initial energy distribution function, the reflection of the electrons from the cathode, the angular distribution of the initial electrons) on the escape coefficient [21].

It was discovered that the initial electron energy distribution is one of the critical parameters significantly affecting the escape factor. The same conclusion is true for the reflection of electrons from the cathode surface, while the angular distribution of the initial electrons has a very small influence on the escape factor. Most importantly, it was found that the range of electrons returning to the cathode exceeds by far the mean free path and that the number of collisions that they make before returning is quite large. The model of cross sections, combined with the selection of realistic initial conditions, las proved to represent the back--diffusion in argon very well, giving good agreement with the available experimental data.

The analysis of the results obtained with our Monte simulation code helps us make relevant conclusions about various characteristics of the back-diffusion process:

- Monte Carlo simulation technique is ideal for studying the back-diffusion of electrons;
- Reflection of electrons from the cathode surface reduces the number of back-diffused electrons and it is relatively observable at low values of the reduced field *E/N*;
- At low values of the initial energy, the escape factor f_{es} depends slightly on the reflection coefficient *R*. The dependence is much greater at higher values of the initial energy;
- For all values of the reflection coefficient *R* (except for *R*=1) the escape factor f_{es} decreases as the initial energy increases;
- When the initial electron distribution is broadly overlapping with low energies, then the nonlinear dependence of the escape factor on the initial energy induces significantly larger escape factors;
- It was found that the anisotropy of the initial distribution does not change the final results very much, so that there is no large difference from the case when all electrons leave the cathode at the right angle;
- When the appropriate values of the distribution function and the reflection coefficient are used, the results of our Monte Carlo simulations show very good agreement with the experimental measurements;
- The semi-empirical formula cited by Phelps and Petrović (8) gives satisfactory values of electron escape coefficients for argon and may be used in determinating the secondary electron yield;
- However, the analysis of our results allow us to point out that the Thomson-Loeb formula (3) cannot be applied to argon even when the exact data of the Monte Carlo code are used.

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Modelovanje procesa povratne difuzije elektrona

Proučavan je efekat povratne difuzije elektrona na katodu primenom Monte Carlo simulacije. Osnovni cilj izvršenih proračuna je bio nalaženje minimalnog seta parametara potrebnog za simulaciju procesa povratne difuzije elektrona kako bi se ova pojava opisala na najjednostavniji način u složenim modelima kolizionih plazmi. Dobijen i rezultati pokazuju odlično slaganje s odgovarajućim eksperimentalnim podacima i mogu se koristiti za proučavanje i predviđanje svojstava procesa pražnjenja koji se javljaju u tehnici naparavanja tankih slojeva, u tehnologiji procesa bitnih za proizvodnju plazma ekrana i lasera, u tehnologiji integrisanih kola, kod detektora nuklearnih čestica itd.

Ključne reči: **povratna difuzija, refleksija, energijska raspodela, Monte Carlo simulacija.**

Modélisation du procès de la diffusion de retour des électrons

L'effet de la diffusion de retour des électrons sur la cathode est étudié par la simulation de Monté-Carlo. Le but primaire des calculs était de trouver l'ensemble minimal de paramètres nécessaire pour la simulation du procès de la diffusion de retour des électrons afin de décrire ce phénomène d'une manière la plus simple possible dans les modèles complexes des plasmas. Les résultats obtenus démontrent le bon accord avec les données expérimentalles et ils peuvent être utilisés pour l'étude et la prédiction des propriétés du procès de décharge se produisant dans la fabrication de plasmas et de lasers, dans la pulvérisation de surface par le bombardement ionique, chez les détecteurs de particules nucléaires, dans la microélectronique, etc.

Mots-clés: **diffusion de retard, reflexion, distribution d'énergie, simulation de Monté-Carlo.**