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SWARM STUDIES ON ELEMENTARY PROCESSES IN NITROGEN

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Nitrogen is widely used in many technical and industrial applications. Electron swarms in a gas under the influence of an electric field can be simulated with the help of a Monte Carlo method. The evaluated swarm parameters are compared with experimental results for drift velocity, electron mean energy and the ionization coefficient. The electron-molecule collision cross sections adopted in the simulation result are in a good agreement with the experimental values.

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1. *Introduction*

Metallic surface nitriding, which produces a thin surface layer having high resistance properties, is applied to improve surface properties such as resistance to corrosion, hardness, wear or fatigue. Nitrogen is the main component of air, and is widely used in many technical and industrial applications. It is abundant, cheap, inert, non-toxic, non-flammable and unquestionably environmentally acceptable. Nitrogen is effective in slowing down electrons, i.e., it is a good electron thermalizer. It has been the subject of extensive studies, partly because of its dominant presence in the atmosphere and its use in gas discharge and gas dielectric applications.

A detailed knowledge of electron swarm parameters in gases are necessary for accurate simulations for plasma processes, such as those used for plasma chemical vapor deposition (CVD), reactive ion etching (RIE) and laser-induced ablation. Typically, electron swarm parameters are used in fluid simulations of plasmas to determine the time-dependent evolution of densities of radicals and charged particles. In particular, they are needed to solve the continuity equation for electrons which includes drift, diffusion and electron multiplication processes. Therefore, investigations of the basic processes in nitrogen-containing plasmas have their own significance. In addition, the transport coefficients and microscopic properties of gases are currently subjects of growing interest to applied research workers in the field of high-voltage insulation. Although these have proved useful for practical purposes, a more accurate and more general description is needed in the context of new gaseous insulators. Such a description is based on micro-physical material properties and collision cross sections. Its primary advantage is to provide a basis for qualitative prediction of the insulating properties of gases and gaseous mixtures [1 – 5].

Monte Carlo simulations have become increasingly important as a tool, particularly in the area of low-temperature plasma physics. Monte Carlo simulation of electron drift in a uniform electric field has the advantage that the motion of electrons at all stages during their passage in the discharge is traced. Also, it is relatively easy to develop the Monte Carlo method in hydrodynamic as well as non-hydrodynamic regimes [6 – 9]. The electron transport in a gas under the influence of an electric field can be simulated with the help of a Monte Carlo method from an initially number of seed electrons. These electrons are treated from their creation until their disappearance out of the domain of the simulation region or by specific collisional processes. The simulation is stopped when all primary electrons as well as the secondary electrons (created, for example, by ionization) are treated. In this paper, the motion of electrons in nitrogen in uniform electric fields is simulated using a Monte Carlo technique.

2. Simulation method

The Monte Carlo method, as applied to the gas discharge problem, involves evaluating the percentage of a given species of particles emanating from a given source, after experiencing energy loss and gain, which terminate in defined categories. In a spherical coordinate system, a background gas of nitrogen molecules with a number density of 3.29×10^{22} m^{-3} which corresponds to a gas pressure of 133 Pa at 20C is considered. The applied electric field E is antiparallel to the z-axis. n_0 electrons with a constant energy are injected from the origin of the coordinate system, assuming a cosine distribution for the angle of entry with respect to the z-axis. The scattering is assumed to be isotropic in the laboratory coordinate system.

The null collision technique has been used [10]. The null collision method is computationally very efficient. The method is useful in calculating swarm parameters in a uniform electric field. The probability of collision and the nature of collision are determined by comparison with computer-generated random numbers uniformly distributed between 0 and 1, at the end of each step.

The new position and energy of the electron are calculated according to the equation of motion. If a collision is not observed, the direction is adjusted according to the parabolic orbit of the electron. When a collision occurs between an electron and a gas molecule, the electron looses the energy corresponding to the type of collision. However, in the case of an ionizing collision, after subtracting the threshold energy, the remaining energy is evenly ascribed to the two electrons. All electrons in the swarm moving forward and backwards, including the electrons formed during the ionization process, are traced until the termination time.

3. *Results and discussion*

In the Monte Carlo technique, the electron trajectories are calculated and collisions of electrons with molecules in the gas are simulated. During the successive collisions, certain information (velocity, position, etc.) is stored for every electron in order to calculate, by appropriate sampling methods, the transport coefficients. The swarm parameters are obtained after following seed electrons from initial conditions for a long period of distance or time. In this paper, we use E/N which has the dimension of $\mathrm{V\,m^2}$. To avoid large negative powers of 10, a unit of 1 Td = 10^{-21} $\mathrm{V\,m^2}$ is used. The employed cross-section set for nitrogen is that given in Refs. [11 − 13].

Under zero-field conditions, Figs. 1, 2 and 3 show the drift velocity, the mean electron energy and the longitudinal and transverse diffusion coefficients. One of the most important validity tests of the treatment of low-energy electron–molecule collisions with Monte Carlo method is to determine transport coefficients under zero-field conditions.

For electrons injected into the gas in a direction, the initial direction of velocity is lost and the electron mean energy relaxes towards gas energy after relatively

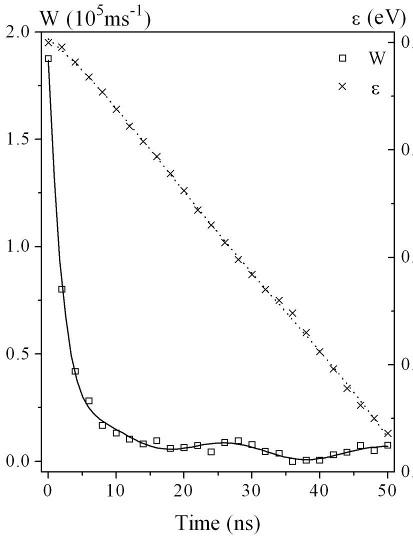

Fig. 1. Zero field electron mean energy (ϵ) and drift velocity (W) as a function of time, for initial electron beams of 0.1 eV *emitted in the forward direction.*

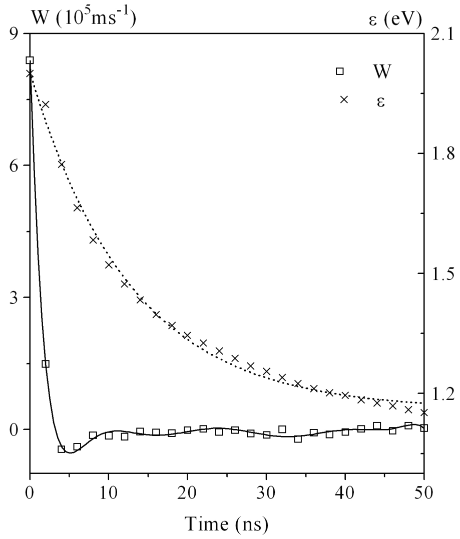

Fig. 2. Zero field electron mean energy (ϵ) and drift velocity (W) as a function of time, for initial electron beams of 2 eV *emitted in the forward direction.*

few collisions. The longitudinal diffusion coefficient, after an overshoot effect, tends towards transverse diffusion. Figs. 1 and 2 show the drift velocity and the electron mean energy of electrons injected in the forward direction, with initial energy of 0.1 and 2 eV.

We are often confronted with a lack of swarm parameters for electrons, especially for the longitudinal diffusion coefficient, when we attempt to simulate the plasma processes in reactive gases. Figure 3 shows the longitudinal and transverse diffusion coefficients for electron beams of initial energy 2 eV and 0.1 eV, injected in the forward direction. In this short time scale, the longitudinal diffusion coefficient, after an overshoot effect due to the anisotropy of the initial distribution, tends towards transverse diffusion.

Figures 4, 5 and 6 show the electron mean energy (ϵ) and drift velocity (W) as a function of time (10 Td), on a shorter time scale, for electrons emitted in the forward direction, with initial energy of 0.1 eV and 2 eV, and the reduced electric field of 10 Td. After relatively few collisions, electrons lose their initial anisotropic angular distribution so that the initial direction of velocity is rapidly lost. The electron mean energy relaxes towards the same energy irrespectively of the initial electron energy (lower or higher than this energy). For a lower initial electron-beam energy (0.1 eV), the longitudinal and transverse diffusion coefficients increase, and the fluctuation is pronounced for the case of the reduced electric field of 10 Td. After that the longitudinal diffusion coefficient, after an overshoot effect, tends towards transverse diffusion. And for the case of $E/N = 0$ Td, on a shorter time scale, the

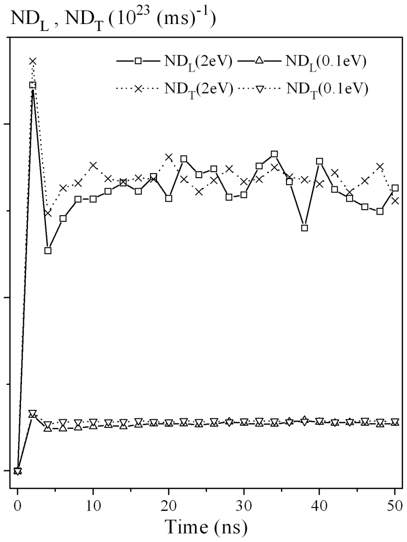

Fig. 3. Zero-field longitudinal and transverse diffusion coefficients, for initial electron beams of 0.1 eV *and 2* eV *emitted in the forward direction.*

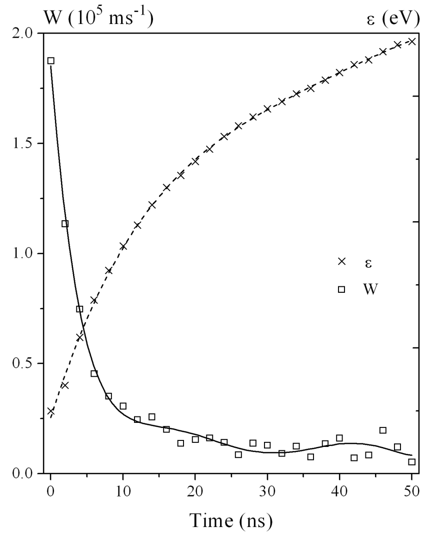

Fig. 4. Electron mean energy (ϵ) and drift velocity (W) as a function of time (10 Td*), for initial electron beam of 0.1* eV *emitted in the forward direction.*

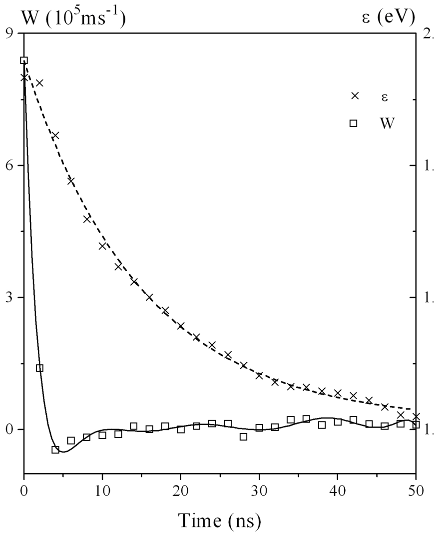

Fig. 5. Electron mean energy (ϵ) and drift velocity (W) as a function of time (10 Td*), for initial electron beam of 2* eV *emitted in the forward direction.*

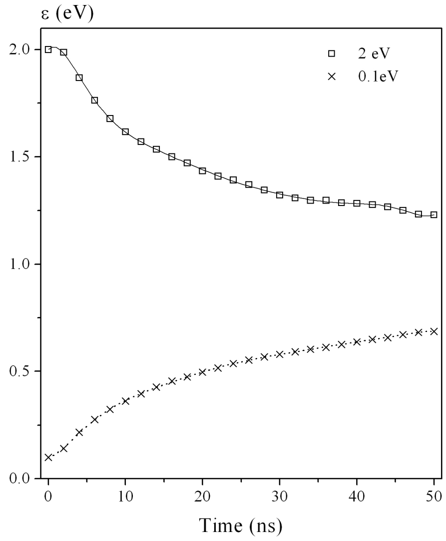

Fig. 6. Electron mean energy: $E/N =$ 10 Td*, with initial electron beam 2* eV *and 0.1* eV *emitted along the forward direction.*

longitudinal diffusion coefficient tends towards transverse diffusion coefficient (Fig. 7).

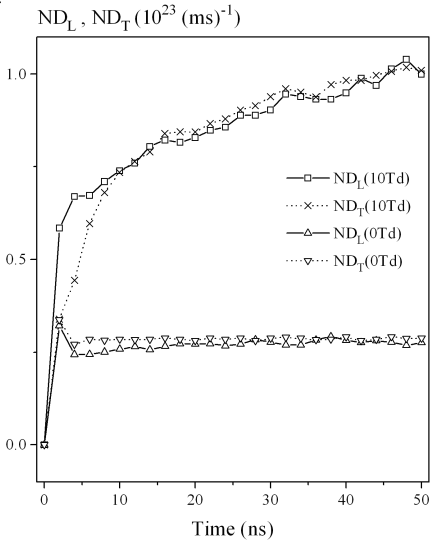

Fig. 7. Longitudinal and transverse diffusion coefficients: $E/N =$ 10 Td *and 0* Td*, with initial electron beam 0.1* eV *emitted along the forward direction.*

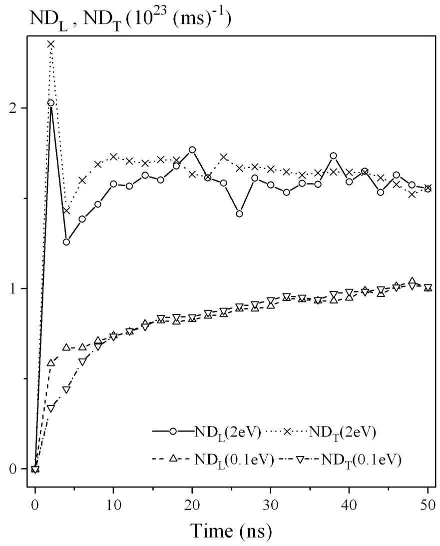

Fig. 8. Longitudinal and transverse diffusion coefficients, with initial electron beam 2 eV *and 0.1* eV *emitted along the forward direction (10* Td*).*

For $E/N = 10$ Td, the longitudinal and transverse diffusion coefficients for the case of initial electron energy of 2 eV are higher than for 0.1 eV, as shown in Fig. 8. In both cases, they tend towards certain values, and in a short time, the longitudinal diffusion coefficient, after an overshoot effect due to the anisotropy of the initial distribution, tends towards the transverse diffusion coefficient.

For a lower value of reduced electric field, the fluctuation of the transport coefficients in the first time scale is attributed to the non-equilibrium of the electron energy distribution. The fluctuation in the latter is attributed to the statistical scatter since the nitrogen is effective in slowing down electrons, i. e. it is a good electron thermalizer. To reduce the scatter, it was thought that a considerable number of electrons need to be injected into the drift space in order to reduce the fluctuation.

Figures 9 and 10 show the variation of electron mean energy, and also ionization coefficient with time for different E/N values. The initial electrons are injected with a mean energy of 0.1 eV. This energy is low enough to influence negligibly the behaviour of the swarm at later times. A time is required for the drift velocity, electron mean energy and ionization coefficient to reach their steady states values. t_0 is the time required for the average electron energy to reach its steady state value. Figuers 11 and 12 show the time variation of the ionization coefficient α, the electron drift velocity and the average electron energy ϵ for the reduced electric field of 600 Td. There is a time lag between the onset of steady state for the average energy and the onset of steady state for the ionization coefficient. The transient in α occurs because initially, at $t \sim t_0$, the number of accumulated ionizing collisions is small, hence the ionization coefficient has not reached its steady state.

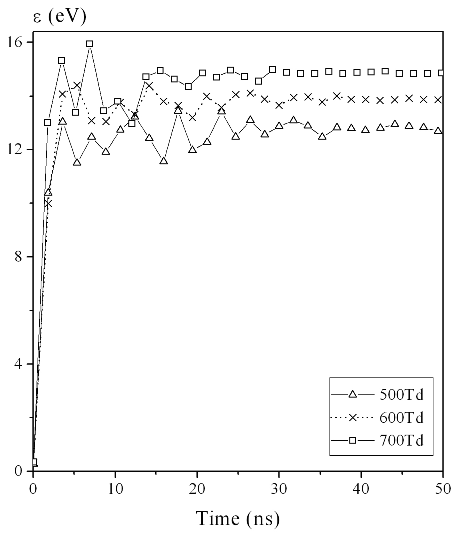

Fig. 9. Mean energy electron as a function of time, for different E/N values.

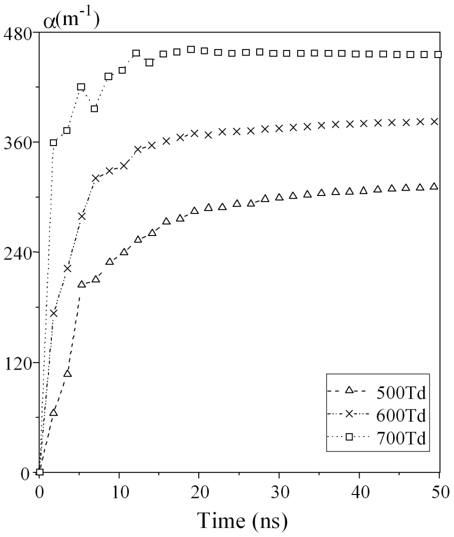

Fig. 10. Electron ionization coefficient as a function of time, for different E/N values.

Figures 11 and 12 also show that the mean electron energy fluctuates, with diminishing amplitude of fluctuation (that is due to the assumed small number of electrons in the avalanche in order to reduce computational costs). The drift velocity, has the same qualitative time behaviour as α, but reaches steady state in a shorter time.

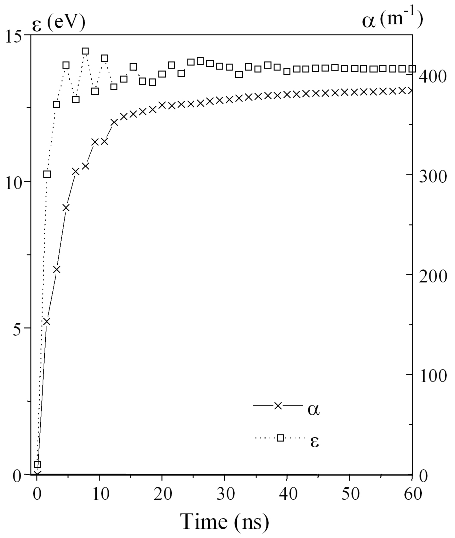

Fig. 11 Mean energy electron ϵ and ionization coefficient α as a function of time, $E/N = 600$ Td.

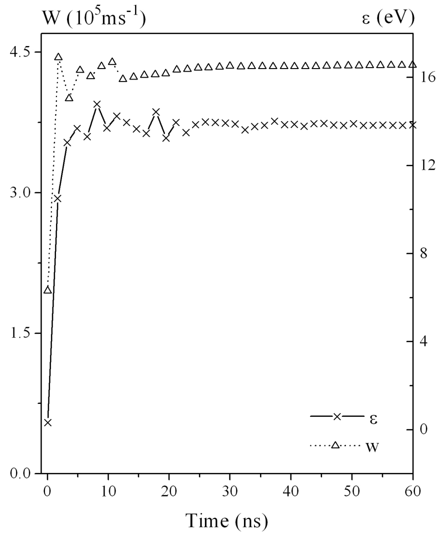

Fig. 12. Mean energy electron ϵ and electron drift velocity W as a function of time, $E/N = 600$ Td.

Figures 13 and 14 show the variation of the electron drift velocity and the mean electron energy, as a functions of E/N. There is a good agreement among the data for drift velocity [14−17] and mean energy [14−16] from various experiments and the values calculated by the Monte Carlo method. The experimentally determined electron drift velocities, using pulsed the Townsend method [18], within the range 10 Td $< E/N <$ 500 Td agree quite well with the present results. The calculated drift velocities with Monte Carlo method compared with the calculated values on the basis of the Boltzmann equation in the two term approximation, in a steady-state Townsend discharge, within the E/N range of 30 Td to 550 Td [19], show a fairly good agreement. The electron drift velocities [20], determined using the pulsed Townsend method, for the reduced electric field values in the range 270 Td to 365 Td agree well with our results calculated using the Monte Carlo method. The present data agree well with the values of the electron drift velocity measured with the pulsed Townsend technique in Ref. [21] over the range of the reduced electric field strength E/N from 50 to 360 Td. The good agreement between experimental data and the simulation results shown in Figures 13 and 14 indicate that the collision calculations accurately predict the growth of electron pulses into electron avalanches.

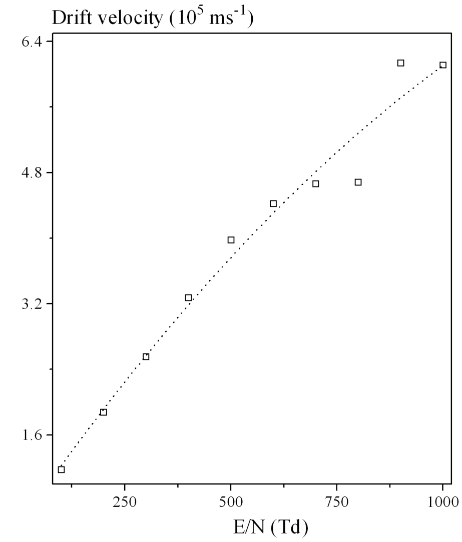

Fig. 13. Electron drift velocity as a function of E/N, fitted curve is the dashed line.

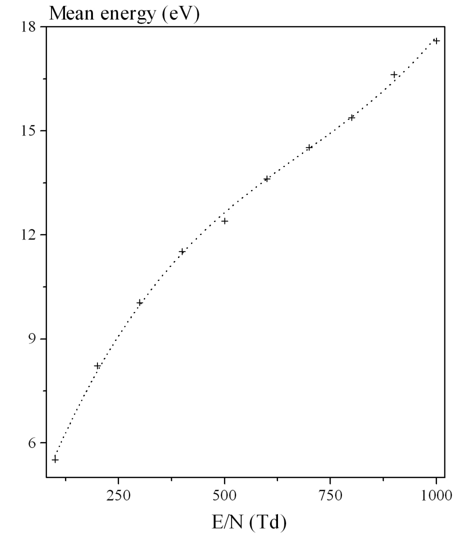

Fig. 14. Mean electron energy as a function of E/N, fitted curve is the dashed line.

In view of practical importance to the engineers, the swarm parameter α/N (reduced ionization coefficient) generated by the simulation technique in this gas is shown in Fig. 15. Reasonable agreement has been obtained between the calculated and measured ionization coefficient [14−17, 22−24]. The experimentally determined ionization coefficients using the pulsed Townsend method [18], within the range 10 Td $< E/N <$ 500 Td, agree quite well with the present results. A good agreement is found between the calculated ionization coefficient with Monte Carlo method, and the calculated values on the basis of the Boltzmann equation under the two-term approximation, in a steady state Townsend discharge. within the E/N range of 30 Td to 550 Td [19]. The present data agree well with the values of the ionization coefficient measured with the pulsed Townsend technique referred in [21] over the range of the reduced electric field strength E/N from 50 to 360 Td. The values of α/N are related to E/N according to the semi-empirical equation

$$\frac{\alpha}{N} = A \exp\left(\frac{B}{E/N}\right) , \tag{1}$$

where A and B are constants characteristic of the gas. For a set of n particles and a given simulation time, the particle energy distribution function (or electron energy distribution function) can be determined. The electron energy distribution function at $E/N = 400$ Td is shown in Fig. 16. The dot lines and full lines show the Maxwellian distribution at the corresponding mean energies. The energy distributions obtained by the simulation indicate Maxwellian tail behaviours at corresponding mean energies.

The agreement between the present calculated distribution functions and the results obtained by Taniguchi et al. [25] is good. The Monte Carlo method is realistic because a large number of particles are followed from the source through their life history. From the history of each species, the average properties are obtained by an efficient tracing method and compared with the respective measured quantity.

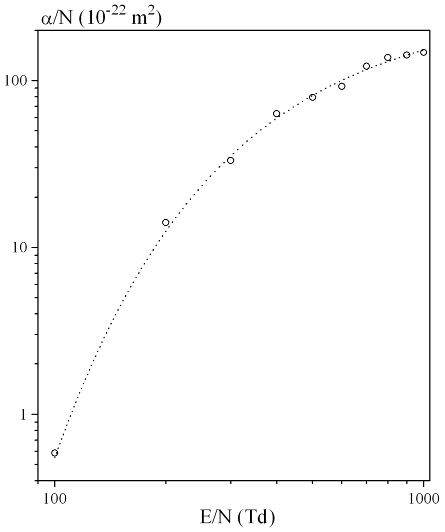

Fig. 15. Reduced ionization coefficient α/N as a function of E/N, curve from equation 1 is the dashed line.

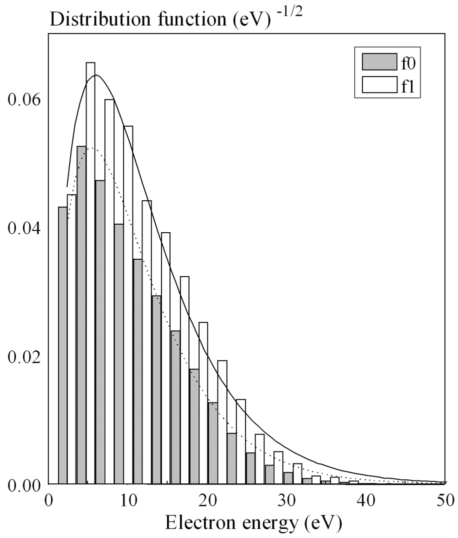

Fig. 16. Electron energy distribution function at $E/N = 400$ Td, f0: isotopic part, f1: with anisotropic parts.

4. Conclusion

Monte Carlo simulations have become increasingly important as a simulation tool, particularly in the area of low-temperature plasma physics. In this study, we have examined the behaviour of electrons in uniform electric fields using a Monte Carlo simulation. Electron swarm parameters were calculated as a function of reduced electric fields E/N. Binary collisions of electrons with neutral gas molecules are the essential mechanism in electron avalanche growth. The simulation results give values for electron drift velocity, electron mean energy, ionization coefficient, longitudinal and transverse diffusion coefficient and electron energy distribution as a functions of time and reduced electric fields. The good agreement between the calculated and measured swarm parameters demonstrates the validity of the binary collision simulation techniques.

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PROUČAVANJE ELEMENTARNIH PROCESA U ROJEVIMA U DUŠIKU

Dušik je u širokoj upotrebi u mnogim tehničkim i industrijskim primjenama. Rojevi elektrona u plinu pod djelovanjem električnog polja mogu se oponašati Monte Carlo metodom. Postignuti rojni parametri uspoređuju se s eksperimentalnim rezultatima za posmične brzine, srednje energije elektrona i ionizacijske koeficijente. U računima prilagođeni udarni presjeci za sudare elektron – molekula u dobrom su skladu s eksperimentalnim podacima.