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A model of dc glow discharges with abnormal cathode fall

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A model for an abnormal glow discharge, including a self-consistent analysis of the cathode fall, was developed. It combines microscopic particle simulation by means of Monte Carlo methods with a fluid model of the gas discharge. The model allows calculations of the steady-state electrical field distribution, the charged-particle densities, and the current densities along the axis of the discharge. The model was used to simulate a glow discharge in 80% He and 20% SF_6 at a pressure of 8 Torr with a current density of 1 A/cm^2. The computed discharge voltage agrees well with measured values. The computer code can easily be modified to describe the charged-particle densities and energies not only in the cathode fall region, but in any plasma boundary layer.

I. INTRODUCTION

Research on glow discharges has been increased strongly in the last decade, stimulated by applications such as gas lasers, high-power switches, plasma processing, and plasma chemistry. Although glow discharges are used extensively, the theory of these discharges is incomplete. Especially the boundary layers in high-current-density (abnormal) glow discharges are poorly understood.

Glow discharges are spatially characterized by three regions: the cathode fall with the negative glow, the positive column, and the anode fall. The anode fall serves to generate the positive ions needed to provide for quasineutrality in the adjacent positive column. Its potential is usually of the order of the magnitude of the ionization potential of the gas atoms or molecules, but it can be increased by decreasing the active area of the anode. The positive column is a plasma region extending between anode fall and negative glow. It is characterized by a constant electric field along the discharge axis. This field is necessary to force electrons and ions to drift through this region, and to provide for ionization and detachment rates sufficient to compensate for charge carrier losses through recombination and attachment. The cathode fall with negative glow is the most important and least understood part of the electrical discharge. It is the region with the highest ionization rate which provides for current continuity to the positive column. It is characterized by a nonhomogeneous field intensity, with its maximum value at the cathode surface, and a more or less linear decrease towards a small value in the layer between cathode fall and positive column, the negative glow.

There are numerous efforts to model glow discharges.[1] The discharge models are based on a description of the electron and ion kinetics coupled with Poisson's equation. The major objective is to calculate the transport and rate coefficients for the charge carriers. These coefficients depend on the local velocity distribution, which is a function of the electric field distribution. In order to simplify the modeling procedure, it is generally assumed that the local velocity distribution, and consequently the transport and rate coefficients, depend only on the local electric field. The value of these coefficients can, therefore, be obtained by measurements or calculations in uniform electric fields. This assumption is called "local field approximation" or "equilibrium approximation," since it implies that the charge carrier kinetics is in equilibrium with the local electric field.

This equilibrium approach has been successful in providing a basic insight in normal glow discharge behavior, discharges with low current, and has proved to be sufficient to explain most of the features of the discharge, even the most complicated part of the discharge, the cathode fall. The cathode fall parameters predicted by the numerical models of Ward,[2] Davies and Evans,[3] and Boeuf[4] are in agreement with experimental data for normal cathode falls.

Local field approximations become questionable when the variations of the electric field over an electron mean free path are large. This is typical for glow discharges with abnormal cathode fall, where currents with densities of more than 1 A/cm^2 are carried. In the abnormal dc glow discharge, the whole cathode is active, and any increase in the discharge current consequently causes an increase in current density. The rise in discharge current density is accompanied by a rise of the cathode fall voltage V_c and a diminution of the cathode fall thickness d_c. In the cathode fall region, the electric field can reach values of tens of kV/cm and varies so rapidly in space that it is no longer permissible to assume equilibrium of the charged particles with the local electric field. The nonequilibrium behavior of electrons in the cathode fall region has been studied by Boltzmann equation analysis and by Monte Carlo simulations. Information about most of these efforts can be found in reviews by Segur *et al.*[5] and Davies.[1] A third method, the convective scheme method, has been recently used to model the electron kinetics in the cathode fall with a self-consistent electric field.[6]

A hybrid model for the positive column and the abnormal cathode fall of a glow discharge is described in this paper. The electron kinetics is modeled by means of a Monte Carlo code, and the computed electron drift velocity and the rate coefficients for ionization and attachment are used in a fluid model to find the charge density and the current den-

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sity distributions of ions and electrons along the discharge axis. An iterative procedure allows us, in addition, to obtain a self-consistent solution for the cathode fall region. The self-consistent calculation is started by guessing an electrical field distribution in the cathode fall region and then computing by means of a Monte Carlo code the spatial distribution of ionization and attachment rate coefficients and the average electron velocity. These data are used to calculate, by means of a fluid model, the charged-particle distributions and, subsequently, using Poisson's equation, a corrected electric field distribution. This field distribution is then used again in the Monte Carlo codes. In order to obtain a self-consistent solution for the discharge, this computational process is repeated until sufficient conformity between subsequently calculated electric field profiles is reached. In order to test this model versus experimental results, it was used to simulate a 1 A/cm^2 linear glow discharge in a mixture of 80% He/20% SF_6 at a pressure of 8 Torr.

II. MODEL

A one-dimensional glow discharge between two infinitely extended plane parallel electrodes is considered. This is a reasonable approximation for abnormal glow discharges where the electrode distance is small compared to the discharge dimension perpendicular to the electric field direction. Furthermore, it was assumed that the discharge is in a steady state, which means that all variables are just functions of position x and do not vary with time. The model is based on numerical solutions of fluid equations and Poisson's equation. The first set of equations are the continuity equations for electrons, and positive and negative ions. They are of the form

$$\frac{d}{dx}(n_i\bar{v}_i)=\sum_j R_{ij}, \tag{1}$$

where n_i is the particle density of type i, $\bar{v}_i$ is the average velocity of these particles, and R_{ij} stands for gain and loss rates, respectively, for the specific kind of particles. For electrons ($i=1$), e.g., the rates which were considered in our model are ionization ($j=1$), detachment ($j=2$), attachment ($j=3$), and recombination ($j=4$). By multiplying the equations with the charge of the particular particles and by adding Eq. (1), the continuity equation for the total current density is given as

$$\frac{dJ}{dx}=0, \quad \text{with } J=e\sum_i Z_i n_i \bar{v}_i, \tag{2}$$

where e is the electron charge, and Z_i is the charge number of species of type i. The total current density is not dependent on position x, but only on the current densities J_i of the different charge carriers.

The second set of equations are the momentum-conservation equations:

$$n_i\bar{v}_i=n_iu_i-\frac{d}{dx}(D_in_i), \tag{3}$$

where u_i is the drift velocity, and D_i is the diffusion coefficient for the ith species of charge carriers. The remaining equation which needs to be solved is Poisson's equation:

$$\frac{dE}{dx}=\frac{e}{\epsilon}\sum_i Z_i n_i, \tag{4}$$

where E is the electric field intensity, and ϵ is the dielectric constant. For a gas discharge which contains electrons and one kind of positive ion, the system consists of five equations for the five unknown spatially dependent quantities: electron density, ion density, average electron velocity, average ion velocity, and electric field intensity.

What needs to be known in order to solve this system of equations are the rate coefficients, and the drift velocities and diffusion coefficients for all types of particles as a function of position x. Furthermore, five boundary conditions have to be used to solve this set of five first-order differential equations.

A. Positive column

The first step in modeling of the discharge is done by describing the positive column. This part of the discharge is characterized by a uniform distribution of charge carrier densities and current densities. Equation (1) is reduced to the form

$$\sum_j R_{ij}=0, \tag{5}$$

which means that gain and loss processes cancel each other at any position x. Second, the average velocity is identical with the drift velocity

$$\bar{v}_i=u_i, \tag{6}$$

and third,

$$\sum_i Z_i n_i=0, \tag{7}$$

which is the quasineutrality condition for plasmas. The homogeneity of the positive column allows to use a zero-dimensional Monte Carlo code to calculate the electron energy distribution with the electric field intensity as a variable parameter. From these data, we obtain the rate coefficients for the various electron-neutral collisions and the electron drift velocity. The drift velocities of the ions were assumed to be proportional to the local electric field intensity E:

$$u_i=\mu_iE, \tag{8}$$

with μ_i being the mobility. By means of Eqs. (5)–(8) for the different types of charged particles, the charge carrier densities and the current densities in the positive column can then be calculated. These results allow one to obtain the value of the total current density as a function of the electric field intensity or, in other words, the current-voltage characteristics of the positive column of a gas discharge.

B. Cathode fall

The computed charge carrier densities and the current densities in the positive column serve as boundary values for the cathode fall region. In this region the carrier densities and the current densities vary in space. The sum of the current densities carried by the different charge carriers, however, is constant, because a one-dimensional system is considered. In order to model this region, the set of differential equations (1), (3), and (4) has to be solved. Because of the spatial dependence of all the rate coefficients and average velocities, a one-dimensional Monte Carlo code was used to determine these parameters as a function of position for the electrons. To perform this simulation the electric field distribution in the cathode fall region has to be known. Unfortunately, in glow discharges with high current densities (abnormal glow discharges), it is not permissible to use the local field approximation in the cathode fall region. Because of strong variation of the electric field intensity in an abnormal (high current density) cathode fall, the electron velocity distribution at a position x and so the rate coefficients k_{ij} and the average electron velocity $\bar{v}_e$ are not just functions of the local electric field, but depend on the field distribution in the vicinity of this position. It is therefore not possible to use the rate coefficients and electron drift velocity as functions of the local electric field, as has been done for the positive column.

For the cathode fall, an iterative procedure has been used to solve for the particle densities and current densities with Monte Carlo simulation of the electron kinetics in an iteratively corrected electric field distribution. The procedure used to obtain a self-consistent solution for the cathode fall was the following.

(a) An arbitrary electric field distribution $E(x)$ in the region between the cathode surface $x = 0$ and an assumed value of the cathode fall distance $x = d_c$ was used as initial distribution. The only condition for $E(x)$ is that it matches at $x = d_c$, the previously computed electric field intensity in the positive column.

(b) A one-dimensional Monte Carlo code was used to find the electron energy distribution, the electron collision frequency, the average electron velocity, and the rate coefficients for electron-neutral particle collisions as a function of position. The initial electron energies at the cathode surface were assumed to be distributed homogeneously between zero and an upper energy value. The electrons were followed over a distance greater than d_c, up to a value of x_0, where the calculated rate coefficients and transport parameters became constant and assumed the positive-column values.

(c) The charged-particle densities and the current densities for the given electric field $E(x)$ were obtained as functions of position by solving the continuity equations and the momentum-conservation equations. The ions were assumed to be in equilibrium with the local electric field[7] and the contribution of the diffusion term to the average velocity was assumed to be negligible. The momentum conservation equation for ions was therefore reduced to

$$\bar{v}_i = u_i = \mu_i(E)E. \tag{9}$$

The average velocity for electrons was obtained from the Monte Carlo calculations. The integration of the set of differential equation (1) was performed in steps of $d_c/10\,000$ from a position of x_0, where the rate coefficients and transport parameters had assumed the positive-column values, towards the cathode at $x = 0$. The charged-particle densities and their average velocities in the positive column were used as boundary values at x_0.

(d) During the integration process, the electron and positive-ion current densities were monitored. The integration was terminated when the ratio of electron current J_e to positive-ion current J_{i^+} had reached a value which corresponds to a given second Townsend coefficient γ. This implies that the electron generation at the cathode surface is due to ion impact only, and that the number of electrons generated per ion (second Townsend coefficient) is not dependent on ion energy. This assumption is reasonable for ion energies below 1000 eV.[8]

(e) The value of x where the condition for the ratio of electron current and ion current is satisfied ($J_e/J_{i^+} = \gamma$) must be the cathode surface. The known charge carrier densities in the range between this newly defined cathode surface and the positive column determine the electric field distribution in this range. By means of Poisson's equation, the electric field intensity $E'(x)$, with $E'(x_0) = E_{d_c}$ as a boundary condition, is calculated and compared with the previously used field distribution $E(x)$. If the difference between the initial field $E(x)$ and the calculated field $E'(x)$ for any x is larger than a given margin, then the described computation is repeated with $E'(x)$ as initial electric field. The procedure (a)–(e) is iterated until a sufficient agreement between successively computed electric field distributions is obtained.

III. MODELING OF A DISCHARGE IN He:SF$_6$

The model was applied to simulate a discharge in a mixture of He and SF_6 at a pressure of $p = 8$ Torr. This gas mixture was chosen because experimental results on the voltage-current characteristics of He/SF_6 discharges were available. This allowed testing of the model what the total voltage, the sum of the fall voltages, and the voltage across the positive column concerns. The electron-SF_6 and the electron-He collision cross sections are relatively well known.[9,10] Cross sections were not available for processes where two of the colliding particles are charged particles. An example is electron-ion recombination. This process and other electron-ion or ion-ion processes, although not considered in the Monte Carlo code, were taken into account in the fluid model, by using reasonable values for their respective rate coefficients. The choice of most of these coefficients is based (roughly) on considerations of recombination processes in diffuse discharges.[11] For the electron-He^+ recombination, a value of 10^{-8} cm^3/s was used; the electron-SF_6^+ recombination coefficient was chosen to be 4×10^{-8} cm^3/s. The rate coefficients for ion-ion recombination were assumed to be 2×10^{-7} cm^3/s for recombination of SF_6^- ions with SF_6^+ ions, and 10^{-8} cm^3/s for recombination of SF_6^- ions with He^+ ions. The rate coefficient for electron detachment from SF_6^- was assumed to be 5×10^{-7} cm^3/s. Because of the low degree of ionization in the gas, the aforementioned processes influence the electron energy distribution only slightly. The accuracy of the rate coefficients for charged-particle collisional processes is therefore not very critical for the discharge simulation.

A. Positive column

The anode fall voltage was not calculated, but assumed to be of the order of 20 V, which is about the mean value of the ionization potentials of the two gases, He and SF_6. As will be shown, this voltage is small compared to the cathode fall voltage and the voltage across the positive column in our simulated discharge. The positive column was modeled in the way described in the previous section. A zero-dimensional Monte Carlo code was used to obtain the electron energy distribution, the collision frequency, the electron drift velocity, and the rate coefficients for ionization and attachment, as a function of the electric field intensity. All scattering processes were assumed to be isotropic. It was also assumed that the energy after an ionizing collision was shared equally between the two outgoing electrons.

The procedure for the computation of the rate and transport coefficients is shown in Fig. 1 in the form of a flow diagram. The "null collision method"[12] was used to reduce the computing time. The number of collisions for one simulation was 10^6. The comparison of the results of this calculation with calculations with different collision numbers showed that the statistical error in the Monte Carlo results is less than 5%.

The results of the Monte Carlo simulations in the positive column are shown in Figs. 2–4. The effect of the electric field on the electron energy distribution is shown in Fig. 2, where energy distributions for electric field intensities of 250 and 400 V/cm are plotted. In Fig. 3 the electron collision frequency and the electron drift velocity are plotted versus electric field intensity. Both quantities increase linearly with electric field intensity E in the range of 250 V/cm $< E <$ 400 V/cm. The rate coefficients for ionization and attachment are shown in Fig. 4. The attachment rate coefficient decreases with increasing electric field intensity. This is due to the strong decrease of the SF_6 attachment cross section with electron energy. With increasing electric field the number of low-energy electrons, which have a high probability to be attached to SF_6 molecules, decreases (see Fig. 2), and so does the attachment rate coefficient. Ionization, on the other hand, increases strongly with increasing electric field intensity, as expected from the influence of the electric field on the electron energy distribution.

In order to find the equilibrium electric field, which is the field where charged-particle gain and loss processes balance each other, the set of fluid equations (5)–(7) has to be solved. For a mixture of two gases, one of them an electro-

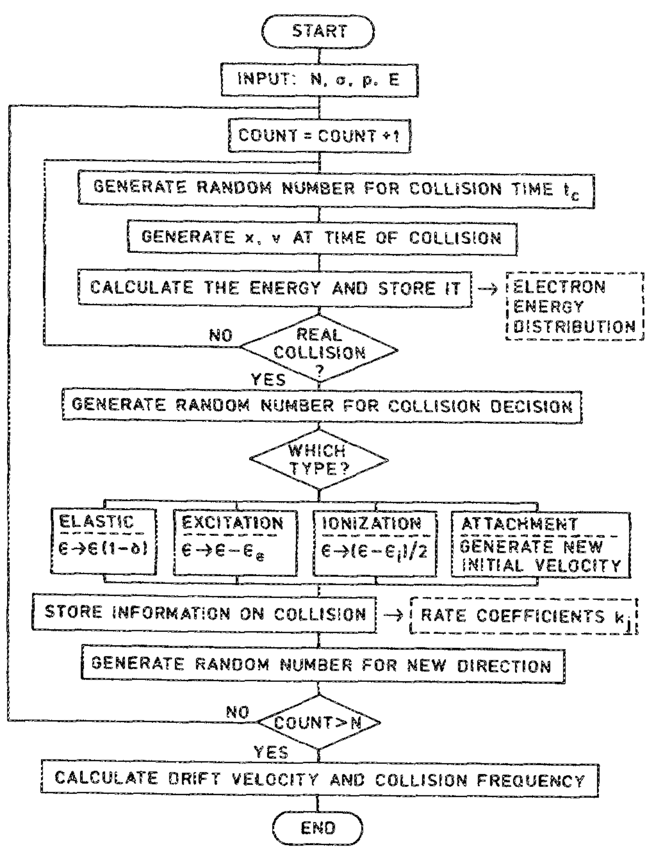

FIG. 1. Flow chart for the Monte Carlo simulation of the electron motion in the positive column of a glow discharge. N: number of collisions; σ: cross sections; p: gas pressure; E: electric field intensity; x: position of electron; v: velocity of electron; ϵ: energy of electron; δ: fractional energy transferred during elastic collision; ϵ_e: excitation energy; ϵ_i: ionization energy.

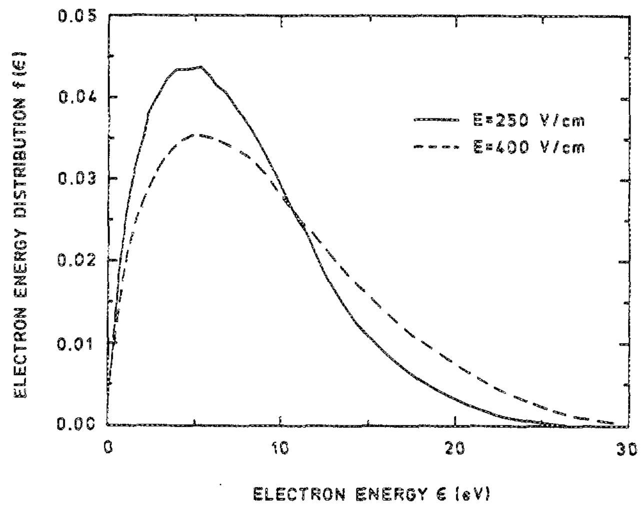

FIG. 2. Electron energy distributions in the positive column of an 80% He/20% SF_6 glow discharge at a pressure of 8 Torr. The parameter is the electric field intensity.

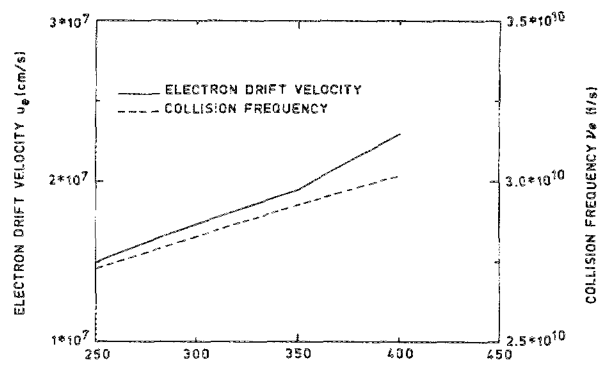

FIG. 3. Electron drift velocity and electron collision frequency as a function of the electric field intensity in the positive column of a He/SF_6 glow discharge.

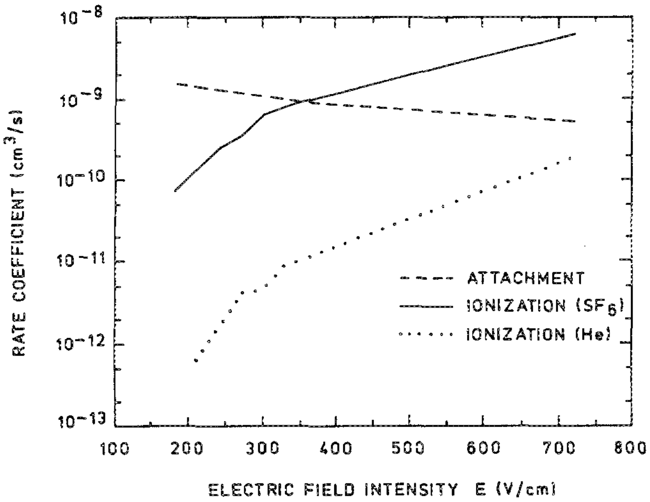

FIG. 4. Ionization and attachment rate coefficients as a function of the electric field intensity in the positive column of a He/SF$_6$ glow discharge.

negative gas, there are at least four types of charge carriers: electrons, negative ions, and singly charged positive ions for either gas. There are therefore four continuity equations, four momentum-conservation equations, and Poisson's equation, which is reduced for the positive column to the quasineutrality condition.

Listed below are the equations used to describe a steady-state glow discharge in 80% He and 20% SF$_6$. For the positive-column simulation, the spatial derivatives are set to zero:

$$\frac{d}{dx}(n_e\bar{v}_e) = 0.8k_{iH}nn_e + 0.2k_{iS}nn_e - 0.2k_a nn_e - k_{rH}n_{H^+}n_e - k_{rS}n_{S^+}n_e + k_d n_{S^-}n_e, \quad (10a)$$

$$\frac{d}{dx}(n_{H^+}\bar{v}_{H^+}) = 0.8k_{iH}nn_e - k_{rS}n_{H^+}n_e - k_{rSH}n_{H^+}n_{S^-}, \quad (10b)$$

$$\frac{d}{dx}(n_{S^+}\bar{v}_{S^+}) = 0.2k_{iS}nn_e - k_{rS}n_{S^+}n_e - k_{rSS}n_{S^+}n_{S^-}, \quad (10c)$$

$$\frac{d}{dx}(n_{S^-}\bar{v}_{S^-}) = 0.2k_a nn_e - k_{rSH}n_{H^+}n_{S^-} - k_{rSS}n_{S^+}n_{S^-} - k_d n_{S^-}n_e, \quad (10d)$$

$$\bar{v}_{H^+} = \mu_{H^+}E, \quad (10e)$$

$$\bar{v}_{S^+} = \mu_{S^+}E, \quad (10f)$$

$$\bar{v}_{S^-} = \mu_{S^-}E, \quad (10g)$$

$$\frac{dE}{dx} = \frac{e}{\epsilon}(n_{S^+} + n_{H^+} - n_{S^-} - n_e). \quad (10h)$$

The average electron velocity $\bar{v}_e$ is obtained from the Monte Carlo calculation. In Eqs. (10a)–(10h), v_{H^+} and

TABLE I. Charge densities and current densities in the positive column of an 80% He/20% SF$_6$ glow discharge at a pressure of 8 Torr.

Charge density (10^{11} cm^{-3})		Current density (A/cm^2)	
Electrons	1.4	Electrons	0.39
He$^+$ ions	42	He$^+$ ions	0.16
SF$_6^+$ ions	39	SF$_6^+$ ions	0.15
SF$_6^-$ ions	80	SF$_6^-$ ions	0.30

v_{s^+} are the average velocities of the He$^+$ ions and the SF$_6^+$ ions, respectively, and v_{S^-} is the average velocity of the negative SF$_6^-$ ions. The electron density is denoted as n_e, the densities of the He$^+$ ions and the SF$_6^+$ ions are n_{H^+} and n_{S^+}, respectively, n_{S^-} is the density of the SF$_6^-$ ions, and n is the gas density of the He/SF$_6$ mixture. The rate coefficients for electron attachment to SF$_6$, k_a, and the ionization coefficients for He and SF$_6$, k_{iH} and k_{iS}, were obtained from the Monte Carlo simulation. The rate coefficient for electron-He$^+$ recombination, k_{rH}, for electron-SF$_6^+$ recombination, k_{rS}, for electron detachment, k_d, and the ion-ion recombination coefficients for SF$_6^-$–SF$_6^+$ recombination, k_{rSS}, and for SF$_6^-$–He$^+$ recombination, k_{rSH}, were assumed to be constants. Because ion diffusion was neglected, the average velocity of the ions is the drift velocity. It is dependent on the electric field intensity through the mobility. The values for the ion mobility for He and for SF$_6$ were chosen according to data listed in Ref. 13. The mobility of SF$_6^-$ ions and SF$_6^+$ ions in He was assumed to be the same.

Solving the fluid equations (10) gave a value of 330 V/cm for the equilibrium electric field in the positive column of an 8 Torr, 80% He/20% SF$_6$ glow discharge. The corresponding charge densities and current densities are listed in Table I. The dominant negative-charge carriers are SF$_6^-$ ions. The electron density is less than 2% of the negative-ion density. However, due to their large mobility, the electrons still make the major contribution to the current density.

B. Cathode fall

In order to model the cathode fall region, a one-dimensional Monte Carlo code was used. As for the positive column, all scattering processes were assumed to be isotropic, and the energy after an ionizing collision was assumed to be shared equally between the two electrons. The motion of 10^4 electrons were recorded, starting from their origin at the cathode surface to a distance where the rate coefficients and drift velocity became constant and agreed with the values in the positive column. The electrons emitted at the cathode surface were assumed to have a random distribution of initial energies between zero and 10 eV. This assumption is based on experimental observations of initial energy distributions of electrons generated by He$^+$ impact on molybdenum electrodes.[8]

The initial electric field intensity in the cathode fall region was chosen to be of the following form:

$$E = E_0(1 - x/d_c), \quad \text{for } 0 < x < d_c, \tag{11a}$$

and

$$E = E_{pc}, \quad \text{for } x < d_c, \tag{11b}$$

with E_0 being the electrical field intensity at the cathode surface, E_{pc} is the electric field intensity in the positive column, and d_c is the cathode fall distance. The procedure for the computation of rate coefficients and drift velocity is similar to the one depicted in Fig. 1, except that the electron motion in the electric field is followed over a certain distance, from $x = 0$ to x_0, rather than for a given number of collisions. The spatial resolution was chosen to be $d_c/20$, which means that all electrons recorded in the range of $md_c/20$ to $(m+1)d_c/20$, with m being an integer between 0 and 19, were treated as being in the same spatial position. Because of the relatively small number of electrons (10 000) and the consequently small number of collisions in certain regions of the cathode fall, curve-fitting methods were used to reduce the influence of statistical fluctuations in the rate coefficients along the discharge axis.

The results of the Monte Carlo calculations, the rate coefficients for ionization and attachment, and the electron drift velocity as a function of position for the given electric field are used to solve the set of fluid equations in the cathode fall region. The fluid equations [Eqs. (10)] were solved numerically by using the fifth-order Runge–Kutta method. The integration was performed in steps of $d_c/10\,000$, beginning at a distance x, where the solutions of the Monte Carlo calculation were consistent with the positive-column values. The particle densities n_i and the current densities J_i in the positive column (Table I) served as boundary conditions for the set of fluid equations in the cathode fall.

The calculated ratio of electron current density to positive-ion current density as a function of position x was used to determine the position of the cathode surface. According to our assumption on the electron-emission mechanism at the cathode, the electron current density at the surface is given by the second Townsend coefficient times the positive-ion current density. For our calculation the value of the second Townsend coefficient was chosen to be 0.3. This assumption is based on measurements of He^+ ions with energies below 1000 eV impinging on clean tungsten or molybdenum electrodes.[8] When the condition for the ratio of electron current to ion current is reached, the integration of the fluid equations is terminated, and the x coordinate is transformed so that its origin is at the newly defined cathode surface.

The electric field intensity E in the range adjacent to the cathode is calculated by means of Poisson's equation using the charge density values obtained by solving the fluid equations. This newly computed field generally differs from the initially assumed electric field intensity. It can be assumed, however, that the new solution is closer to the real electric field intensity in the cathode fall than the previous one. The new electric field was therefore used to recalculate the discharge parameters using the same procedure as described above. The computation time for each one of these iterations was 10 CPU hours on a CDC 180 computer.

The solution for the electric field intensity was converging very rapidly. An example is shown in Fig. 5 where the electric field intensity as a function of distance from the cathode surface after different steps of the iteration procedure is plotted. The initial field intensity curve was chosen according to Eqs. (11a) and (11b) with the electric field intensity at the cathode surface being $E_0 = 20$ kV/cm, and the cathode fall distance being $d_c = 0.1$ cm. At distances larger than d_c, the electric field intensity was assumed to be 330 V/cm, which is the computed electric field intensity of the positive column E_{pc}. After two iterations already, the solution for the electric field intensity is stable. The electric field decays towards the positive column monotonically as assumed in most nonself-consistent models. However, it decays, differently from normal cathode falls, hyperbolically rather than linearly. The cathode fall voltage which is obtained by integrating over the electric field distribution from the cathode surface ($x = 0$) to the positive column ($x = d_c = 0.5$ mm) is, in this case, 400 V.

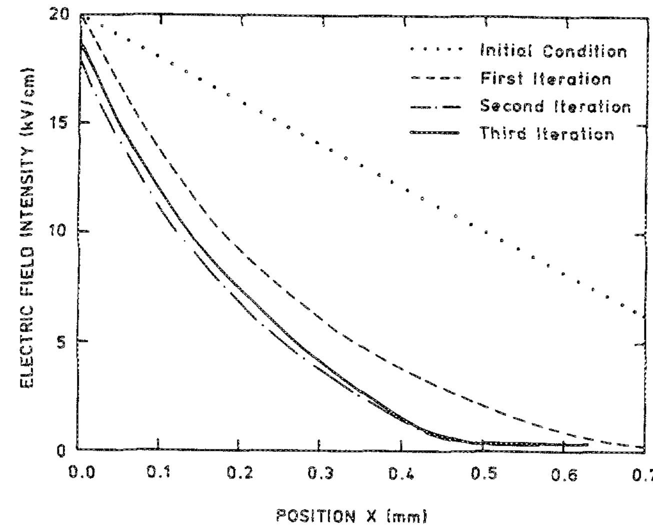

FIG. 5. Computed electric field distribution in the cathode fall region of an abnormal glow discharge in He/SF_6 obtained through an iterative procedure.

Since a self-consistent solution should be independent from the initially chosen conditions, the model was tested by using a different initial electric field distribution, with similar shape as the first one, but with E_0 and d_c being ten times smaller. As shown in Fig. 6, the solution after the second iteration is almost identical with the solution obtained with the first initial conditions.

Knowing the electric field intensity as a function of position allows one to compute the electron energy distribution, and consequently the electron drift velocity and the rate coefficients as a function of position. Figure 7 shows the normalized electron energy distribution in the cathode fall region and the positive column. The electron energy distribution in the region close to the cathode surface (0.05 mm $< x <$ 0.35 mm) does not have a pronounced maximum. There is a relatively large number of high-energy electrons which provide for a high ionization rate in this region. Towards the positive column the number of slow electrons is

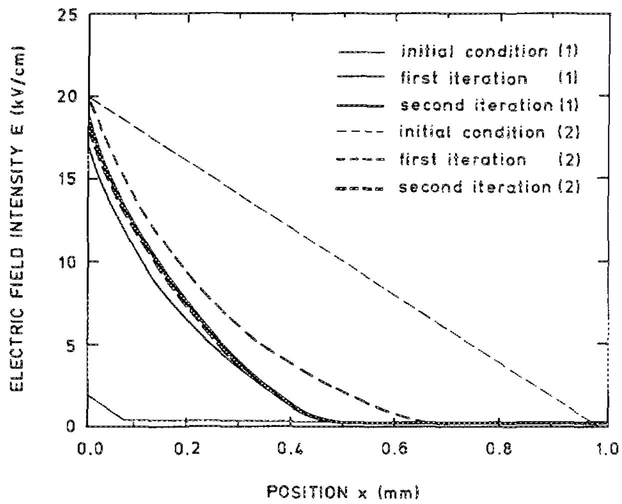

FIG. 6. Computed electric field distribution in the cathode fall region of an abnormal glow discharge in He/SF_6 obtained through an iterative procedure with two different initial conditions.

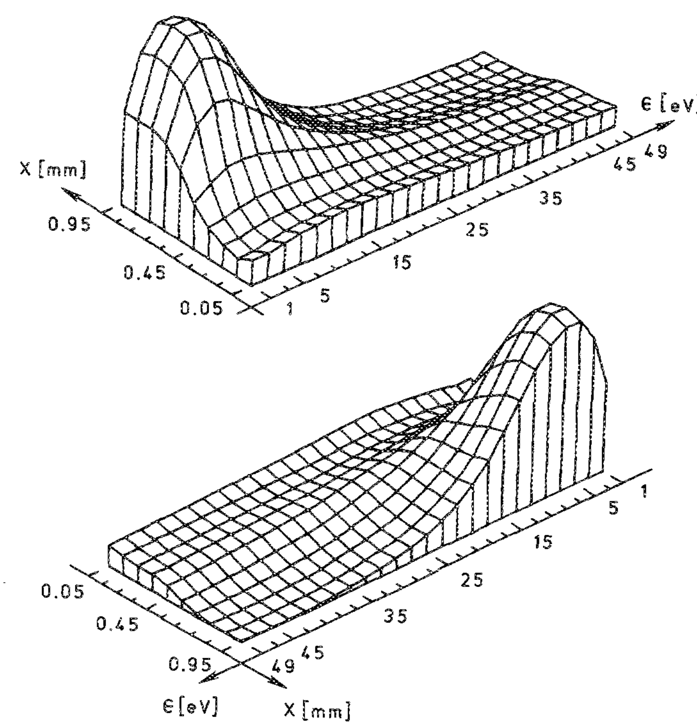

FIG. 7. Normalized electron energy distribution in the cathode fall region seen from the cathode (above) and from the positive column (below) as a function of the distance to the cathode surface.

increasing on the expense of fast electrons. The consequence is that the ionization rate decreases and the attachment rate increases until a full balance of charged-particle gain and loss processes is reached in the positive column. The electron energy distribution is at energies above 20 eV over the entire cathode fall distance a function which is monotonically decreasing with energy. This is different from Monte Carlo results in glow discharges in He, where a second maximum in the energy distribution at higher energies was found.[14,15]

The spatial distribution of the average electron velocity is plotted in Fig. 8. It is about 1.5×10^8 cm/s in the vicinity of the cathode and decays over a distance of 0.4 mm to the positive-column value of 1.8×10^7 cm/s. The rate coefficients for ionization and attachment are shown in Fig. 9. The ionization rate coefficient shows the expected maximum at a distance of about 0.1 mm from the cathode. This clearly demonstrates the nonequilibrium situation: although the electric field intensity has its maximum at the cathode surface, the ionization coefficient does not have a maximum at this position. The attachment rate coefficient also shows this nonequilibrium behavior: it has a minimum where the ionization coefficient has its maximum and rises toward the positive column where it eventually assumes the same value as the reduced ionization coefficient.

The spatial distributions of the rate coefficients and the electron drift velocity are needed to solve the fluid equations and to compute the discharge parameters for the abnormal glow discharge. The charged-particle distributions are shown in Fig. 10 and the current distributions are plotted in Fig. 11. The charge density of negative ions in the positive column ($x>0.5$ mm) exceeds that of electrons by almost two orders of magnitude. This is typical for discharges in strongly attaching gases such as SF_6. The electron density in the cathode fall region ($x<0.5$ mm) is constant up to a distance of 0.1 mm from the cathode surface. The positive- and negative-charge density, however, varies by one order of magnitude over the cathode fall thickness. This is contrary to what generally is assumed for normal cathode falls. Usually the positive-charge density is assumed to be constant over the range of $0<x<d_c$.[16] On the other hand, the electric field distribution which is related to the charge density distribution through Poisson's equation is not drastically different from the one obtained in semiempirical models.

Although the electron density is much smaller than the negative-ion density in both regions, the cathode fall and the positive column, the electron current is still the dominant

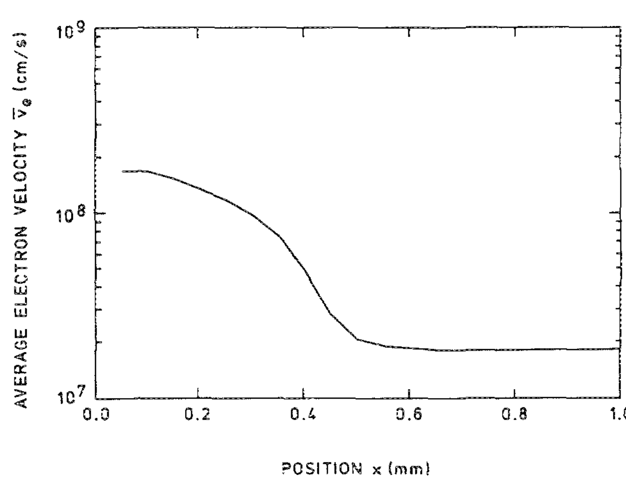

FIG. 8. The average electron velocity vs distance from the cathode in the cathode fall region.

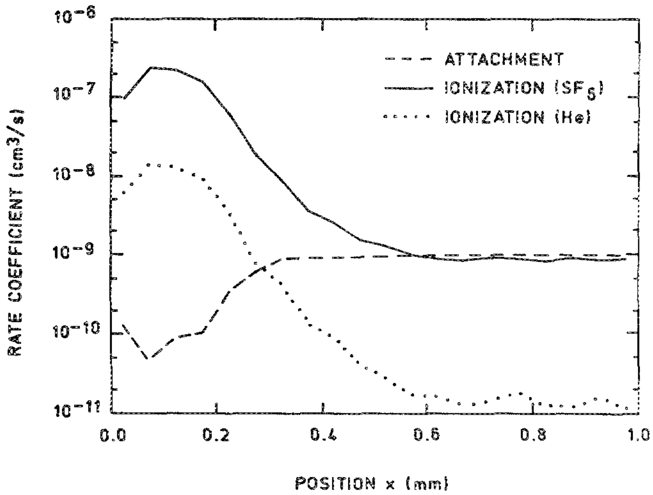

FIG. 9. Ionization and attachment rate coefficients vs distance from the cathode in the cathode fall region.

current in the discharge except for a small layer of 0.1 mm adjacent to the cathode surface. In this region the positive SF_6 ions carry most of the current. The dominance of the positive SF_6 ion current close to the cathode surface can be understood by considering the ionization potential of SF_6 (15.7 eV) compared to that of the He (24.5 eV).

IV. CONCLUSION

The model, which connects microscopic particle simulation with a fluid model, allows one to compute the discharge parameters, such as electric field, particle densities, and current densities in glow discharges. It includes a self-consistent treatment of the nonequilibrium region, the cathode fall. The computational procedure is based on iterative correction of the electric field used in one-dimensional Monte Carlo code for the electron kinetics. Good results were obtained after just two iterations.

The model was used to simulate a glow discharge in a mixture of He and SF_6 (80%/20%) at a pressure of 8 Torr with a current density of 1 A/cm^2. The calculated electric field has its maximum of 18 kV/cm at the cathode surface and decreases hyperbolically towards the positive column, where it reaches its minimum value of 0.33 kV/cm. The electron energy distribution does not exhibit a well-defined group of high-energy electrons, which was found in glow discharges in He experimentally[17] and by means of a Monte Carlo analysis.[14,15] One possible reason for this discrepancy is the assumption of isotropic scattering in our Monte Carlo calculation. Anisotropic angular scattering, which was considered by Boeuf and Marode[15] for elastic collisions in He, can significantly affect the electron energy distribution. The fact that the high-energy component is missing in our results could also be due to the difference in gas composition. Our discharge was operated in a gas mixture where the collision frequency for inelastic processes is dominated by the gas component SF_6, rather than by He. The enhanced collision rate in the He/SF_6 mixture might prevent the development of the group of high-energy electrons found in pure He.

By solving the fluid equations, it was found that the positive-charge density in the cathode fall decreases by one order of magnitude towards the cathode surface. In normal glow discharges, on the other hand, the positive ions are assumed to have a constant density in this region, contrary to what we found for the abnormal discharge. Although the He concentration was four times higher than the SF_6 concentration, the dominant positive-ion density at the cathode surface was the $SF_6{}^+$ density.

The cathode fall voltage was found to be 400 V in this particular discharge. Experiments performed under the same conditions gave values of 1.1 kV for the discharge voltage at current densities of 1 A/cm^2.[18] The gap length in these discharges was 2 cm. Using the computed value of the electric field intensity in the positive column (330 V/cm), which was assumed to span over a value of close to 2 cm, and adding cathode fall and anode fall voltage, gave calculated

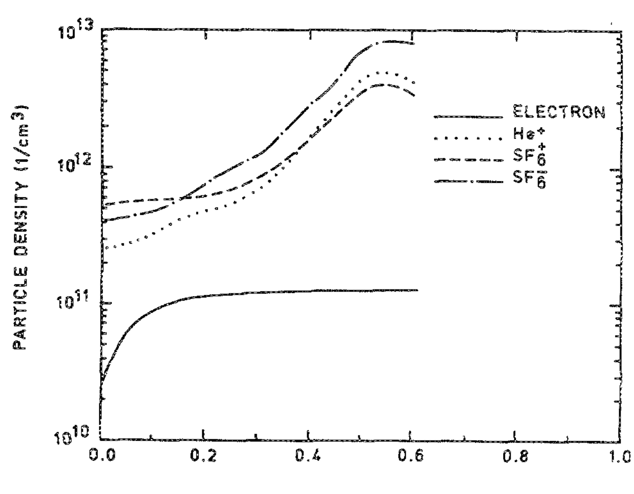

FIG. 10. Charged-particle density distributions in the cathode fall region of an abnormal glow discharge in He/SF_6.

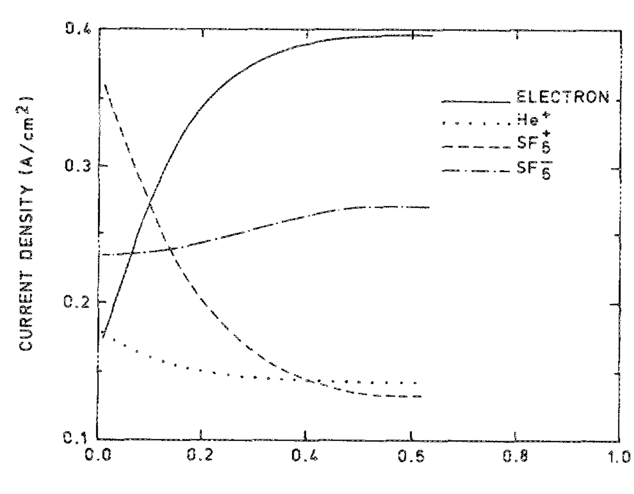

FIG. 11. Current density distributions in the cathode fall region of an abnormal glow discharge in He/SF_6.

values of 1.08 kV for the discharge voltage. Experiment and theory agree well.

The computer code, which was used to describe a discharge in He/SF_6, can be applied to any one-dimensional gas discharge, as long as the basic data of the gases are known. Furthermore, it is not just able to provide a self-consistent solution for the cathode fall of a glow discharge, but it can also be used to calculate particle densities and particle energies in any linear plasma boundary layer. In order to analyze the boundary layer of a glow discharge at the surface of a dielectric, the same procedure can be used as described above. The only difference would be that the condition at the dielectric surface would be of the form $\Sigma_i J_i = 0$ (positive and negative current densities cancel) instead of the Townsend condition valid for the cathode fall. This versatility and the possibility to expand the code easily to high-frequency gas discharges could make it a useful tool in predicting and controlling reactions in surface processing devices.

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