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ON MICROELECTRONICS,
DEVICES AND MATERIALS
and the WORKSHOP on
ORGANIC SEMICONDUCTORS,
TECHNOLOGIES AND DEVICES**



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PROCEEDINGS

**September 28 – September 30, 2011
Ajdovščina, SLOVENIA**

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FOREWORD

Dear colleagues,

Welcome to the 47th International Conference on Microelectronics, Devices and Materials, (MIDEM 2011) and joint Workshop on Organic Semiconductors, Technologies and Devices. This conference continues the tradition of annual international meetings organized by MIDEM - Society for Microelectronics, Devices and Materials, Ljubljana, Slovenia. These conferences have always attracted a large number of Slovene and foreign experts as well as distinguished guest speakers. At the conferences scientists have the opportunity to present their activities and research progress to the international audience and to discuss trends and problems related to their fields of work with other colleagues. This year, 42 regular and 10 invited participants will present their achievements during three days from Wednesday to Friday. The contributions are grouped in 6 conference sessions: Materials, technology and devices, Electronics, Optoelectronics, Thin and thick films, Integrated circuits, Sensors and actuators and in the conference workshop.

This year MIDEM workshop focuses on organic semiconductors (OSs) and related technologies and devices. This exciting field of science and technology is rapidly growing mostly because of the possibility that electronic and optical properties of OSs can be tailored to a particular application by changing chemical composition of the pertinent molecule. In addition OSs promise the fabrication of devices that are compatible with flexible substrates allowing thereby to design optoelectronic devices that are not possible by using inorganic semiconductors. In the past fifteen years the development in this area made great strides, so that we are now faced with first commercial organic light emitting diodes (OLEDs) and displays fabricated on thin, flexible foils. Organic thin film transistors, although not as fast as their inorganic counterparts have also found their position in some organic/inorganic compound devices. Significant progress has been also recorded in the area of organic solar cells (OSCs).

A key to this rapid progress is close cooperation between organic synthetic chemists and physicists. Advanced methods of synthetic organic chemistry result in molecules whose electronic and optical parameters can be matched to a particular device. Both, small-molecule materials and polymers are also compatible with relatively uncomplicated deposition techniques such as dip-coating, spin-coating and even printing. The possibility to fabricate optoelectronic devices by printing opened a completely new way of thinking in electronic industry. For example, large-scale fabrication techniques, coupled with relatively low cost source materials can compensate for the currently lower efficiency and lifetime of OSCs.

The workshop on Organic semiconductors, devices and technologies gathers invited contributions from the leading research groups working on chemistry of advanced organic materials, devices and theoretical treatment of electronic, optical and structural properties of these materials.

We would like to express our thanks to invited speakers and contributors of regular papers for their valuable scientific contributions to the conference sessions and to the workshop. The members of the International Scientific Board of the conference, who made the review of the contributions, are gratefully acknowledged. We also thank the Conference Organizing Committee members who did their best to make the conference successful.

We hope that all of you will enjoy the conference talks and events, and that you will have an interesting and pleasant stay in Ajdovščina.

Ajdovščina, September 2011

G. Bratina, I. Šorli

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Towards Optimisation of Gas Discharge Tubes

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Abstract – The Gas Discharge Tubes (GDT's) represent one class of a wider group of high-power switches and surge protecting devices such as electronic, electro-mechanic, gas surge arresters etc. realisations. Such element serve as reliable electrical resistors with infinite resistivity, physically installed between the ground and certain critical points in the electrical supply networks of civil-engineering objects, so as to act as ideal electrical short-cuts in the occasions of external over-voltages, capable to bear extremely high currents with, on one hand, very prompt response to unwanted values of over-voltage and, on the other hand, having as short as necessary relaxation time back to ideal resistor state. In this paper we are interested in the particular question of the effects of external magnetic field to the time-developments of the discharge that might be related to possible optimisation of GDT's, aiming for over-voltage protection against the atmospheric lightning. Method of investigation is numerical simulation based on kinetic modelling of the electron and ion motion in combined electric and magnetic fields.

1. Introduction

The gas discharge breakdown is one of the oldest and one of most exhaustively investigated problem in the history of plasma physics [1], which is still far from being fully understood and described (see e.g., Refs. [2] and [3] and references therein). Due to its high importance for many areas like basic plasma physics, vacuum and material sciences, atomic and molecular physics, technology and engineering applications, it is still a subject of intense research via experimental, theoretical, numerical, and computational methods. The breakdown problem has been tackled via full kinetic model, i.e., via so called Particle in Cell method [3,4] only recently (see e.g., Refs. [3] and [5] and references therein), however, still in some its particular aspects, while further investigations towards full reproduction of experimental data and prediction of new ones is a challenging task waiting to be performed via numerical method in next decades. However, it is expected that first attempts [5] on using kinetic codes will considerably help in further understandings of effects of various physical mechanisms and that kinetic codes will considerably contribute to further optimizations of devices based on electrical gas discharge principles. Such efforts might be very important also for basic physics, technology and engineering applications.

Particle in Cell (PIC) codes found application in modelling and solving the behaviours of e.g., thrusters, plasma display panels, low-temperature processing plasmas [capacitive, inductive, electron cyclotron resonance (ECR)], fluorescent lamps, micro-

wave breakdowns, high power microwave devices, multipliers (single/dual surface), plasma focused beam physics (wakefield, pasotron), magnetically confined plasmas, fusion plasmas, heavy ion fusion, space plasmas, basic plasmas.

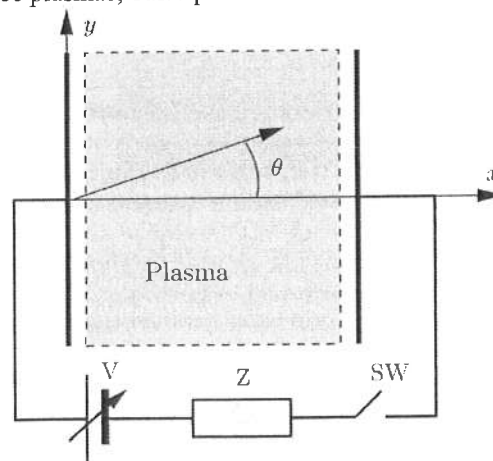


Figure 1: Schematic DC discharge in plane geometry

In this paper we use available versions of free PIC codes known today as PTSG (Plasma Theory and Simulation Group) i.e., Berkeley suite of codes (in particular XOPD1 and XOOPIC [4] codes which are one- and two-dimensional in configuration space respectively, and both three-dimensional in velocity space). While the 1D codes are usually electrostatic, the 2D codes like XOOPIC are based on coupled relativistic particle motion equations with Maxwell equations, subject to given realistic boundary conditions with combined boundary surfaces characterized by a variety of surface physics processes, while at the same

time, the computational domain, which is physically characterised by ionised gas, is a part of an external electrical circuit. Schematic diagram of computational domain between two plane-parallel electrodes is shown in Figure 1, together with external electric circuit and external magnetic field B making angle θ with respect to the electrode surface. The basic diagram showing the principles of PTSG codes with Monte-Carlo collision model is illustrated in a rather self-explanatory flow-chart diagram in Figure 2.

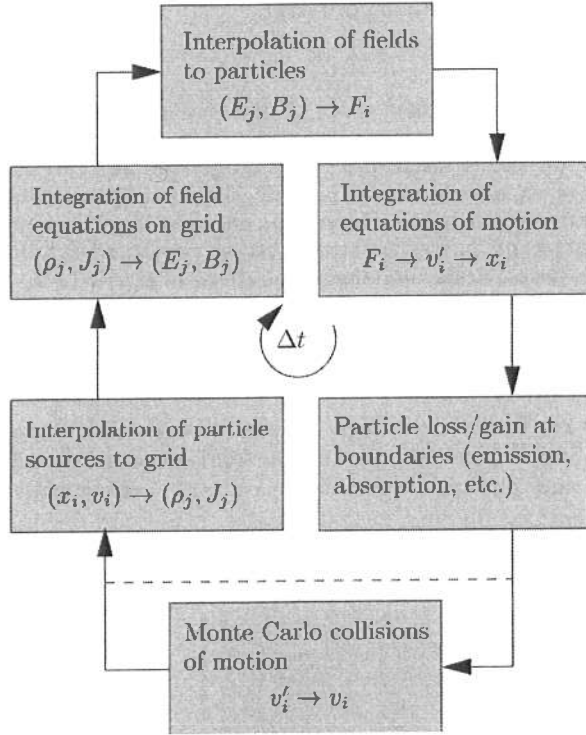


Figure 2: Flow-chart of PTSG PIC codes

Besides the main loop of coupled Newton and Maxwell equations, a fair number of binary collisions calculated via Monte Carlo Collision method (MCC) can be switched on or off, as well as Coulomb collisions for a variety of gases, which, anyway, can be extended to take into account more physics and more gases. Surface processes are taken into account, but need better models to be implemented in near future.

2. Theoretical considerations

There are several basic experimental combination of parameters like e.g., the “ pd ” (pressure times a relevant characteristic dimension of the discharge tube) and “ E/p ” (where E is the electric field) on which the breakdown in gases depend, which follow both from dimensional analysis and experimental results. In a steady state these parameters enter via electron multiplication and via ionisation mechanism. It is assumed that an electron emitted at negative electrode (cathode) accelerated further towards positive anode at position

x , as measured from the cathode, will produce at an elementary distance dx number of dN new electrons proportional to the number N at position x , i.e.:

$$dN = \alpha N(x) dx \quad (1)$$

where α is known as the first Townsend coefficient (or avalanche) coefficient, which corresponds to the inverse effective ionization length. It is in principle not constant but depends on product E/p . For at least several gases it can be approximated by expression:

$$\alpha(x) = p C_1 \exp \left[-C_2 \frac{p}{E(x)} \right] \quad (2)$$

where e.g.,

$C_1 = 5.4 \times 10^{-6} \text{ Pa}^{-1} \text{ m}^{-1}$, $C_2 = 139 \times 10^{-6} \text{ VPa}^{-1} \text{ m}^{-1}$,
 $C_1 = 2.1 \times 10^{-6} \text{ Pa}^{-1} \text{ m}^{-1}$, $C_2 = 25 \times 10^{-6} \text{ VPa}^{-1} \text{ m}^{-1}$,
 $C_1 = 10.2 \times 10^{-6} \text{ Pa}^{-1} \text{ m}^{-1}$, $C_2 = 135 \times 10^{-6} \text{ VPa}^{-1} \text{ m}^{-1}$
 for H₂, He and Ar, respectively, (for more experimental details see e.g., von Engel, Osmokrovic at al 2005). Therefore from Eq. (1) it follows that each electron starting from anode produces in the primary avalanche

$$\frac{N}{N_0} = \exp \left[\int \alpha dx \right] - 1 \quad (3)$$

ions. Providing that each ion which comes back after the first avalanche to the cathode, there initiates emission of γ new electrons due to collision with the cathode surface, so that after sufficient number “ n ” of such cycles the number of ions between the electrodes will be:

$$\frac{N}{N_0} = \exp \left[\int \alpha dx \right] \sum_{k=0}^n [\gamma (\exp \left[\int \alpha dx \right] - 1)]^k \quad (4)$$

or, for sufficiently large number of “cycles”

$$\frac{N}{N_0} \approx \frac{\exp \left[\int \alpha dx \right]}{1 - \gamma (\exp \left[\int \alpha dx \right] - 1)} \quad (5)$$

so it follows that the breakdown will appear for

$$\int \alpha dx = \ln \frac{1 + \gamma}{\gamma} \quad (6)$$

where it has been taken into account that γ is much less than unity in most cases of interest. It should be recognised, that in the case of homogeneous electric field α becomes constant and so formula (6) reduces to

$$\alpha d \equiv p d C_1 \exp \left[-C_2 \frac{p}{E} \right] = \ln \left[\frac{1}{\gamma} + 1 \right] \quad (7)$$

i.e., after substituting relation $E=V/d$ which holds unless the space-charge effect take role

$$pd = \frac{1}{C_1} \ln \left[\frac{1}{\gamma} + 1 \right] \exp \left[C_2 \frac{pd}{V} \right] \quad (8)$$

Furthermore, providing that γ is independent on V , an explicit formula is obtained

$$V = C_2 \frac{pd}{\ln \left[\frac{C_1}{\ln \left(\frac{1}{\gamma} + 1 \right)} \right] + \ln(pd)} \quad (9)$$

Formula (9) is the famous Paschen's law – see e.g., Ref. [1]), holding under above assumptions. It is clear that it holds for enough high pressures

$$pd > \frac{1}{C_1} \ln \left(\frac{1}{\gamma} + 1 \right) \quad (10)$$

and has minimum value for

$$pd = \frac{2.71828 \dots}{C_1} \ln \left(\frac{1}{\gamma} + 1 \right). \quad (11)$$

This minimum value is consequently given by

$$V_{min} = 2.718 \dots \frac{C_2}{C_1} \ln \left(\frac{1}{\gamma} + 1 \right) \quad (12)$$

It is clear that the minimum discharge voltage is rather sensitive to the coefficient γ . For H_2 for example, with above mentioned values we obtain $V_{min} \cong 70 \ln(1/\gamma + 1)$ [V], (otherwise, the multiplicative term in front of logarithm for all gases is several tens, e.g., 50 ± 25) stating that the minimum value could be as low as several tens of volts, providing that the secondary emission is enough high. In practice, it is a fraction of unity, so that in experiments we obtain values of the order of several hundred of volts, meaning that γ is a small fraction of the total number of ions coming to the cathode. This means that in vicinity of the minimum breakdown voltage $(pd)_{min} \approx V_{min}/C_2$ the range of pd -product is of the order of several tenths of $barr \times mm$.

Above considerations are not strictly valid even in homogeneous electric field since γ is in fact intrinsically *not* independent on electric field, as the secondary electron yield depends on the ion incident energy on the cathode. Moreover, in the case when the space charge effects take place, i.e., a plasma forms with a thin sheath, the electric field becomes important as well, so a common formula

$$\gamma = M(V)e^{-G/E} \quad (13)$$

may be employed, providing a kind of surface material-field-ion interaction coefficients $M(V)$ and gas coefficient G are known. Anyway, in this possible situation the whole above analysis should be modified since then neither α might be considered as constant. In any case the extreme importance of γ from above analysis is evident. The best idea would be to find an engineering solution how control this quantity by external means (e.g., hot emitting cathode)!

3. Code benchmarking

Our investigations here are devoted to the initial stage of the breakdown, i.e., before above state is established. This period of breakdown development is characterised by two dynamic stages, i.e., so-called single, or "primary" electron avalanche, and ion current formation stage. We here consider these stages first separately and then analyse their consequences together, as a necessary prerequisite for breakdown being a fully developed quasi-neutral ideally conducting plasma. The computational scenario is roughly as follows: first we prepare the simulation region empty throughout the volume of charged particles with exception of a couple of electrons emitted from the left electrode and "suspended there for the external voltage V to be applied. In $t=0$ the switch "SW" is closed and so a DC voltage is applied, which is in the present examples varying from -200 to -25000V. From that moment electrons are start to move acquiring and interchanging their energy with other particles. The probability for ionization of the external and microscopic electric fields and neutral gas is rather high with respect to other non-elastic binary processes like e.g.,

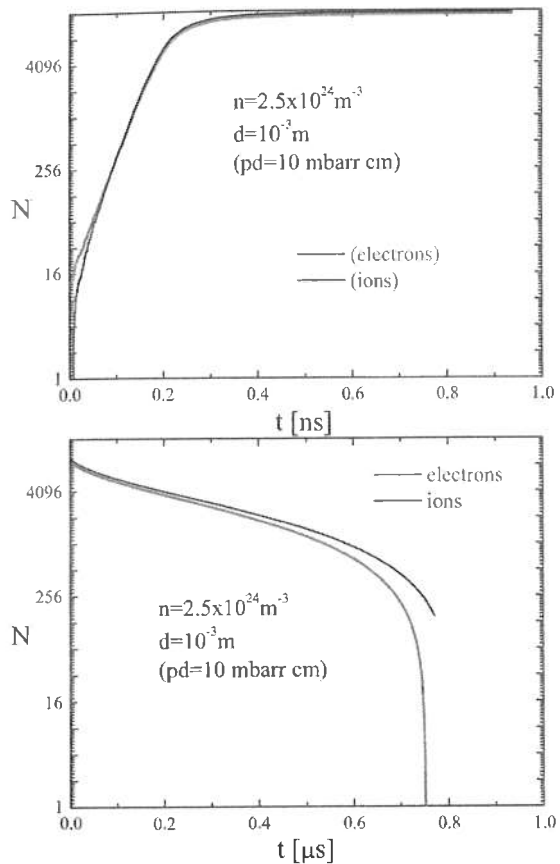


Figure 3: Characteristic times of a primary avalanche stage (top) and plasma relaxation stage (bottom)

charge exchange, excitation, recombination etc., and depends on the gas kind. The gas in present simulation is Hydrogen. In Figure 3 we show the characteristic times of a primary avalanche (top fig.) and the ion and electron (plasma) ambipolar relaxation time, under the conditions as indicated there for H_2 . Shown example represents a rather complex situation with a high particle density where the space charge effects are important, chosen here for investigating if the particle increase is exponential at least in time, as indeed becomes evident in logarithmic presentation of the number of ions and electrons in Figure 3. In Figure 4., however, we show the spatial distribution of the ion density. It is obtained for the case when space-charge might be neglected during a time of the order of one microsecond. Several steps of motion of the ion cluster is presented. The first one is created after a single primary electron avalanche. From this curve it is evident that the simulation confirms perfectly exponential increase of ion multiplication in space. At this moment all the electrons generated in the primary avalanche are already lost at the anode and ions might be regarded as "frozen". On the other hand, all curves there might be regarded as originated from several repetitive primary avalanches. Their duration is shorter than a nanosecond each. If their repetition is enough high, e.g., exactly $0.1\mu s$ this produces within approximately exactly

1 μs (depending on length) an *instant* picture as in Figure 4. In fact, an instant picture will be a superposition of all such instant states.

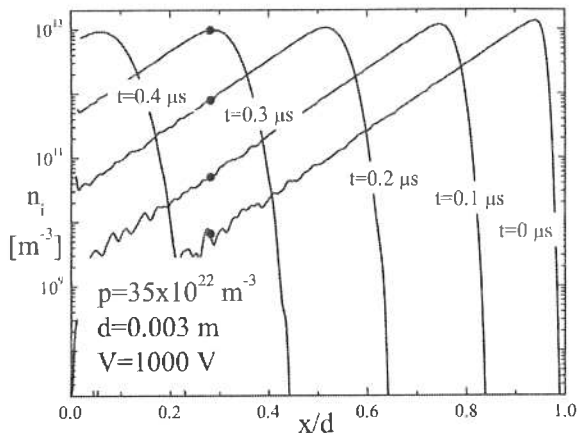


Figure 4: Logarithmic ion density after a single avalanche

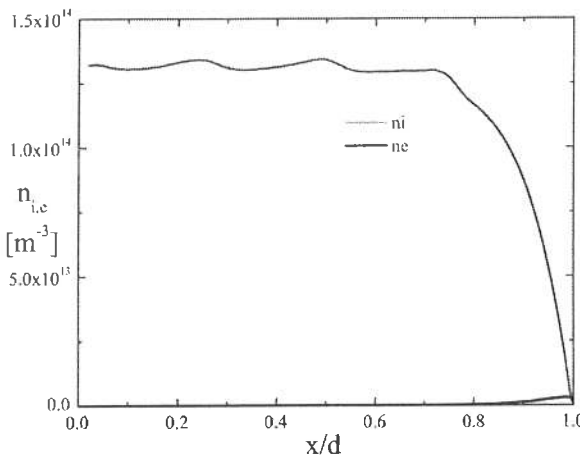


Figure 5: Ion and electron densities in a steady state

This is illustrated in Figure 5 where we show the results of such a superposition of sufficiently high number of single ion shots so as to get result as expected from which in fact correspond to formula (5). We artificially create at the cathode surface roughly 100 electrons in periodic time-steps (one electron at each 10ns) and added all such “frozen” ions for reconstructing the ion distribution which nearly resembles to a developed breakdown. However, it is should be recognized that behind such a practical approach there is a much more complicated theory of particle motion in electric and magnetic fields than above presented. Namely, a steady state, or a breakdown, as first, means that a steady current continuity equation holds, and this can't be satisfied only with ions, since they are not present near the anode so $j = e(n_i u_i - n_e u_e)$, (where e is the elementary charge, $n_{i,e}$ and $u_{i,e}$ are the volume ion and electron densities and average velocities, respectively) has to be satisfied everywhere assuring the absence of inductive term $\epsilon_0 \partial E / \partial t$. This is presented in Figure 5 where the electron density is shown via the

last electron avalanche density distribution. Due to electron high mobility, i.e., velocity, their density in steady state is, obviously, much lower the density of ions.

4. Results

We perform simulation experiments with and without external magnetic field with the motivation that a magnetic field, due to spiral motion of ions and

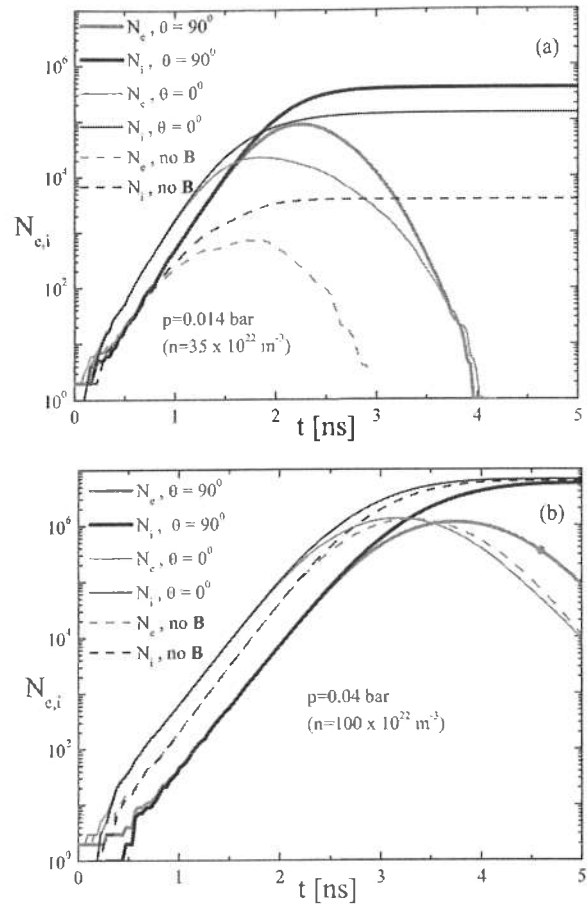


Figure 6: Number of electrons during the avalanche at two different pressures.

electrons, may considerably change their mean-free paths, i.e., the time-life before their escape on boundaries. Under conditions relevant for GDT's the external field does not influence considerable the ion trajectories, but rather the electron motion only. From engineering point of view we find appropriate to employ a magnetic field with strength of $B=0.1\text{T}$ in both convenient for construction directions, i.e., parallel to and normal to the electric field (cases $\theta=0$ and $\theta=90^\circ$). These cases, in comparison with the case without magnetic field applied, are illustrated in Figure 6 where we compare the number of ions and electrons in the discharge region for the cases of two pressures which differ for a factor of roughly three.

However, there are dramatic differences in the charged particle densities in these two cases, which differ for almost two orders of magnitude. This effect seems to be clear, because the total number of the system is exponentially dependent on pd-product and has nothing to do with magnetic field, but the influence of the magnetic field on the number of particles strongly qualitatively differ in these two cases. Namely, while for lower pressure (Fig. 6a) both parallel and perpendicular magnetic fields lead to increased number of ions and electrons (as the angle θ is bigger, the number of particles is higher), for increased pressure (Fig. 6b) both ions and electrons reach the same maximum values. (The only difference in the history of avalanche for higher of two pressures is a slight time-shift appearing as the angle is changed). Simply speaking, the external magnetic field is important for low pd-products but has not effects in the discharge at high pressures!

Furthermore, we investigate the magnetic field effects also in the case when the primary avalanche is started with injected extremely high electron density, when considerable space-charge is formed already during the first primary avalanche. In Figure 7 we present the plasma potential profiles at several different times of the avalanche evolution. In all cases, during the avalanche stage the potential profile quickly changes its profile, so that in a time shorter than $1\mu\text{s}$ it consists of a linear one and a flat region. This flat part corresponds to quasi-neutral plasma and while linear part is a sheath where the whole potential drop is localised. Of course, like in the case with low emission the number of particles will dramatically increase providing additional primary avalanche appear. However, if this happen (and this is our task to control the way how it will happen) plasma will quickly occupy (within the time period of the order of $1\mu\text{s}$) the whole region between the electrodes. The electric field will be concentrated near the cathode in a short region which thickness can be quickly estimated to be:

$$d = 10\lambda_D = 10\left(\frac{\epsilon_0 k T_e}{n e^2}\right)^{1/2} \approx 743 \frac{\sqrt{T_e}}{\sqrt{n_e}} \quad (14)$$

(where in the second engineering expression one has to put the electron temperature in electron-volts and the density per cubic meter) i.e., several so called Debye lengths λ_D . The default value of the electron temperature might be estimated to be of the order of unity, as illustrated in Figure 8 where we show the typical temperatures of ions and electrons during the fast and slow stages of the electron and ion populations developments. Therefore, depending on plasma density the sheath thickness might be estimated to be consequence of such thin well below millimeter and micrometer scales. As a sheath formation an extremely high electric field appears at the cathode, which will cause so-called field-induced secondary electron emission (as described by e.g., formula 13), leading

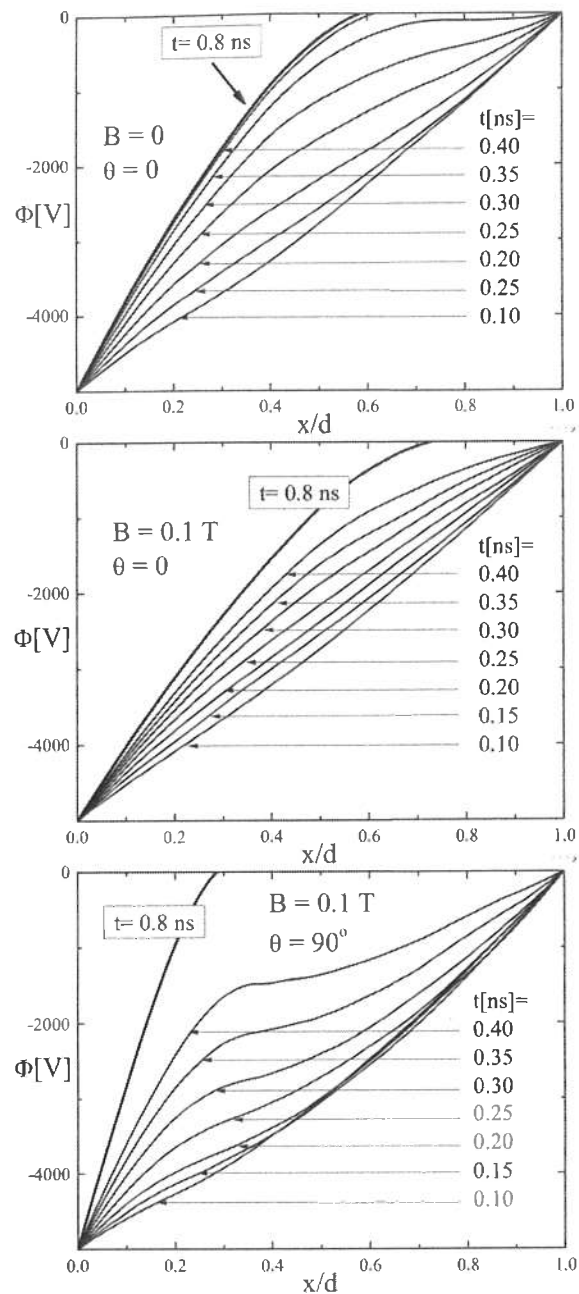


Figure 7: The effects on the magnetic field to the potential profile

further to increase of the plasma density and its conductivity... However, since the plasma is a part of external circuit above described process will not continue indefinitely, but it will be determined by the self-impedance of the GDT and external element Z , as shown in Figure 1. In any case, once the plasma becomes an ideal resistor, the voltage between electrodes will tend to drop to zero, causing a feedback mechanism of decreased plasma density leading back to increased resistivity and thus to increased voltage on electrodes and so on..., but whatever happens, should be enough fast so that the a parallel network does not have time to respond to the lightning stroke

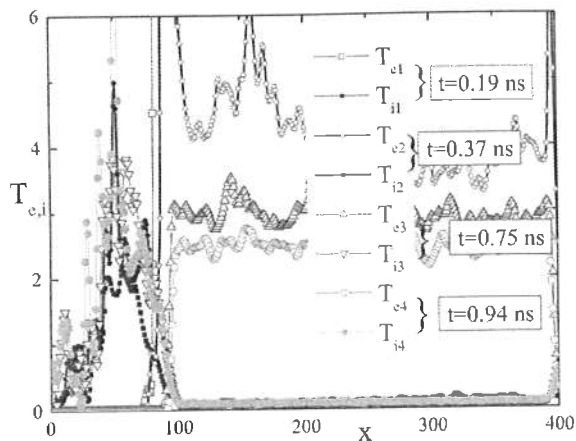


Figure 8: Instant ion and electron temperatures in both slow and fast stages of the discharge

on protective element represented by our discharge chamber. Since the plasma parameters are sensitive to the magnetic field at least at low pressures, this is a possible way how to change the effective pd -product. Here we have shown only a qualitative picture obtained via PIC simulations.

5. Discussion

At lower pressures where binary collisions are negligible, there is none motion of electrons from cathode towards anode since it is entirely determined by the so-called $E \times B$ drift causing spiral motion only in transversal direction. For increased pressure electrons can be "kicked out" from the magnetic field lines due to binary collisions, become capable to diffuse across the magnetic field lines obeying a combined spiral and random motion. Their life-time in magnetic field increases with increased pressure, so probability for gaining additional energy from the electric field between the two collisions, and thus probability for ionization increases. The effect of magnetic field with increased pressure is deleted, so the life-time became independent on magnetic field. This effect opens possibilities to relax the pd -law via introducing an effective length " d " which is dependent on magnetic field configuration and strength. Numerical simulation method is an excellent versatile tool which in combination with experimental method became a very promising one for engineering practice, especially at present times when powerful computation resources became available. The advantage of the method is the possibility to investigate one by one particular physical features of interest, via "switching on" those physical mechanisms which are of interest and "switching off" those ones which might interfere observed phenomenon. In this sense the PIC method is superior over all others including experimental ones, for the simple reason that in experiment such a selectivity of phenomena of interest with other ones waiting in background is hardly

achievable. However, for further employing this rather new approach in applications to breakdown phenomena, we still have to assure that all relevant physical processes will be implemented in existing kinetic and future codes. This is a huge task starting from identifying missing physics in theoretical models as well as in existing codes and then to find and implement proper models into the codes or to write new ones from scratch.

Acknowledgments

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