47th INTERNATIONAL CONFERENCE ON MICROELECTRONICS, DEVICES AND MATERIALS

and the WORKSHOP on

ORGANIC SEMICONDUCTORS, TECHNOLOGIES AND DEVICES

CONFERENCE 2011

PROCEEDINGS

September 28 – September 30, 2011
Ajdovščina, SLOVENIA

PUBLISHED : September 2011
EDITORS : G. Bratina, I. Šorli
PRINTED BY : BIRO M, Ljubljana
PUBLISHED BY : MIDEM
Society for Microelectronics, Electronic Components and Materials
1000 Ljubljana, Stegne 7, SLOVENIA

CIP - Kataložni zapis o publikaciji
Narodna in univerzitetna knjižnica, Ljubljana

621.3.049.77(082)
620.1/.2(082)
681.586(082)

INTERNATIONAL Conference on Microelectronics, Devices and Materials (47 ; 2011 ; Ajdovščina)
Proceedings / 47th International Conference on Microelectronics, Devices and Materials and the Workshop on Organic Semiconductors, Technologies and Devices, September 28 - September 30, 2011, Ajdovščina, Slovenia ; [organizer MIDEM - Society for Microelectronics, Electronic Components and Materials ; editors G. Bratina, I. Šorli]. - Ljubljana : MIDEM - Society for Microelectronics, Electronic Components and Materials, 2011

ISBN 978-961-92933-1-7

1. Bratina, Gvido 2. Workshop on Organic Semiconductors, Technologies and Devices (2011 ; Ajdovščina) 3. Strokovno društvo za mikroelektroniko, elektronske sestavne dele in materiale (Ljubljana)

257579520

The Proceedings of the MIDEM 2011 Conference
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Konferenca MIDEM 2011 in Delavnica o organskih polprevodnikih, tehnologijah in napravah sta delno financirani s pomočjo sredstev Ministrstva za visoko šolstvo, znanost in tehnologijo v sodelovanju z Javno agencijo za tehnološki razvoj v okviru akcije INO-11 (pogodba št. INO-02).

Conference MIDEM 2011 and Workshop on organic semiconductors, technologies and devices are partially financed with subsidy of Ministry of Higher Education, Science and Technology in association with Public Agency for Technology of the Republic of Slovenia within the campaign INO-11 (contract no. INO-02).

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 come 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 advances 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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Particle-in-Cell Simulation Approach to Gas Discharge Tube Study

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Abstract **– The motivation for this work comes from the field of over-voltage/surge protection devices called Gas Discharge Tubes (GDT). GDT's can be installed in all levels of electric power distribution grids with the purpose of over-voltages in cases of atmospheric discharges, short circuits and other malfunctions/natural phenomena. In general they work as perfect high-voltage switches acting as infinite resistors during normal operation and as perfect conductors in case of external over-voltages. The nature of such gas discharge tubes allows them to carry extremely high currents when conducting and the return to their resistive mode when the surge wave passes. Our intention was to study the initial phenomena in that occurs during the breakdown inside the tube, namely the avalanche process in order to better understand it's nature and find a way to optimize the way this class of devices are constructed. This paper deals with the effects of space-charge collected in the simulated area. This happens when the charged particles injected in the domain and additional charged gained through ionization process perturb the electric field enough to make impact on the potential profile and consequently on the avalanche process. This question is also important in the view of field enhanced emission from the boundaries.**

1 INTRODUCTION

Even though there have been extensive and in detail studies of gas breakdowns made over the last 100 years and there is abundant literature on the subject e.g. [1], there is still many new aspects that provide an insight into this phenomena [2]. One of such alternative approaches is also the use of fully-kinetic particle-in-cell (PIC) codes [3]. PIC codes have since the pioneering ideas by Dawson et al. in the early 60's through their well implemented realization later become a relevant and realistic tool for solving (mostly) plasma related problems in numerous fields, e.g. plasma edge physics, fusion plasma, plasma beam physics, thrusters, etc. Since kinetic PIC simulations are real-time simulations coupling Maxwell's field equations with Newtonian mechanics, they allow for a temporal study of discharge phenomena, which is especially important for a research of individual breakdown stages. One of the downsides of PIC codes is, that they are understandably computational very demanding as there are many particle-particle, particle-field and particle-surface interactions, therefore making the selection of relevant parameters crucial. Even though there is many people working in computational physics of plasmas today, there is still only a limited amount of widely obtainable, somewhat benchmarked codes available today. One of the most generally developed and also freely available is the

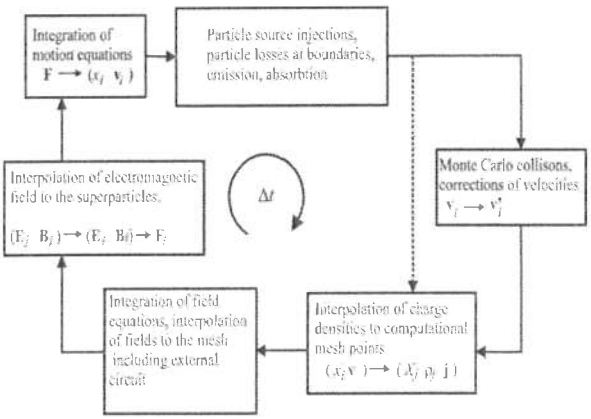

Figure 1: PIC code flowchart

PTSG (Plasma Theory and Simulation Group) suite of codes made at the University of Berkley e.g. XPDP1, XOOPIC [4]. The former is 1d3v (1 spatial dimension, 3 velocity dimensions), while the latter is 2d3v. A In our work regarding space-charge effects we have willfully neglected the effects of added second dimension, as the nature of solving Poisson equation in 2d disallowed us high enough precision needed for our work principle. Our effort being made on a more global scale is however to simulate a realistic gas breakdown by evaluating the effects of particular phenomena in order to get a realistic full size discharge.

2 THE PHYSICS OF BREAKDOWN

The DC discharges considered here falls under category of dark electrical discharges, where number density of excited particles is relatively low, so little light is emitted. In order of current increasing, we can divide it into five divisions, namely: *background ionization, saturation region, Townsend discharge, corona discharges* and lastly *sparking* or *electrical breakdown*. Our interest lies in the region of Townsend discharge, as avalanche process is the most important part of this phenomena. The basic experiment used to study breakdown physics is a rather simple one. Two opposing planar electrodes connected via a high-voltage source are located inside a vacuum chamber. Distance between the electrodes d and the gas pressure p are then varied in order to obtain so called *"Paschen's curves"*, which represent the dependence of the breakdown voltage

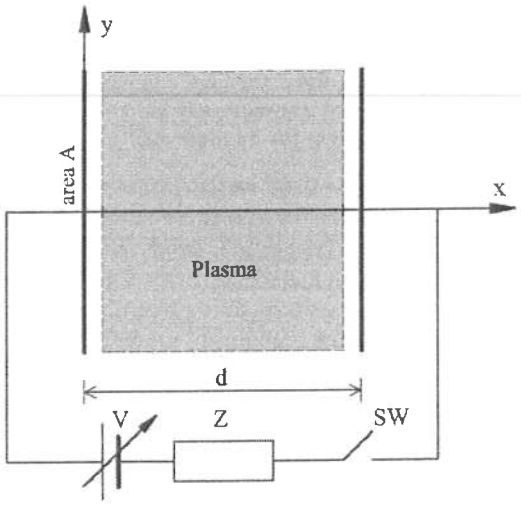

Figure 2: Simulation setup

on the *pd* product. Initially we need some charged particles, which can be provided through a number of processes like photoionization, background radiation ionization, thermionic or field emission etc. These particles then accelerate in the external electric field E_p and can in a certain range of conditions produce additional charged particles through collisional ionization. If the conditions are suitable (E_p, p, d), an avalanche effect occurs and a large number of potential current carriers is produced. This avalanche is generated not only in time, but also in space in DC fields, since the motion of electrons and therefore the ionizations occur predominantly in one direction. The parameter describing the multiplication of electrons is named the *first Townsend coefficient*, denoted by

$$N_e(x) = N_{e0}\exp(\alpha x), \tag{1}$$

where N_{eo} is initial number of electrons at an arbitrary point (e.g. cathode), and $N_e(x)$ is the number of electrons proportional to the distance traveled by the initial electrons. A formula can be written for coefficient α, according to experiments:

$$\alpha = C_1 p \exp\left(-\frac{C_2}{E/p}\right), \tag{2}$$

where $C_{1,2}$ are experimentally determined constants describing gas properties and also taking in account actual effective ionization energy of electrons, since potential energy is also lost through elastic and inelastic (excitation) collisions as well as ionization. For each gas, therefore exists a certain optimum of parameters for ionization. This set of parameters is called the *Stoletow point*, and designates the point of maximum current.

This breakdown itself however is not dependant on avalanche process alone, as a single avalanche is rarely enough for a self-sustained discharge. Additional electrons have to be provided through other processes, mostly through secondary emission due to particle-surface impact and also due to field emission. Losses of particles are provided via diffusion, surface absorption and recombination (dissociative, radiative, ion-ion). A balancing equation can therefore be written in terms of *Townsend criterion*:

$$\ln\left(1+\frac{1}{\gamma}\right) = \alpha d, \tag{3}$$

where γ is *Townsend's second ionization coefficient*, usually referring to the particle-surface interaction, but can also cover other secondary production mechanisms. In most cases, secondary emission is the result of the ion produced in the ionization accelerating towards the cathode and producing (knocking out) an electron upon hitting the surface. This coefficient γ represents the number of electrons emitted per incident positive ion. Secondary processes ensure the reproduction of electrons removed by the field without outside help. This is formally written as *balance (reproduction) coefficient* μ:

$$\mu = \gamma\left(\exp(\alpha d) - 1\right), \tag{4}$$

where the unity of $\mu = 1$ denotes the steady self-sustained current. It can be seen from equation (3), that the electron generation process is highly dependent on secondary emission coefficient γ, If we write down relation

$$E_b = \frac{V_b}{d}, \tag{5}$$

and place it into (3), we obtain an equation for breakdown voltage V_b:

$$V_b = pd\frac{C_2}{\ln\left(\frac{C_1}{\ln\left(\frac{1}{\gamma}+1\right)}\right)+\ln(pd)}, \quad (6)$$

which in fact is the *Paschen's law*. Paschen's law covers well the breakdowns in conditions of low and moderate pressures and not too small distances between gaps, but is subjected to anomalies in micrometer gaps or very high/very low (vacuum) pressures. It can be seen however, that the breakdown voltage is highly dependent on emission coefficient γ, and a sharp boundary between modes can be drawn in the balance equation. When secondary processes actually begin, we have a number of back-and-forth cycles of electron emissions due to ion impact followed by avalanche processes and electron losses. Of course we cannot speak of a gas breakdown when we only have a microscopic self-sustained current. While a formative time of breakdown is a question of definition, an occurrence of exponential current growth over time followed by a macroscopic current is a requirement. As long as the space charge accumulated in the gap between electrodes is not high enough to disturb the external electric field, we remain in the dark (Townsend) discharge process. When this happens, however, a region of quasi-neutral plasma occurs in which the electric field tends to zero. As no field for acceleration of charged particles is available, the avalanche ionization process is soon shut down in this region. We also get a distinctive regions ranging from the electrodes to the quasi-neutral region, namely cathode layer and anode layer. As there is no potential drop occurring in the plasma region, the whole potential difference is now concentrated only on the cathode layer, which can represent only a few percents of gap size. The potential drop on the anode side is much smaller and is usually at least a hundred times smaller than the cathode region voltage drop. The discharge regime transitions from dark to glow discharge by this time. We can usually describe these two boundary regions using plasma physics terminology and refer to them as sheaths, since space-charge build up results in the Debye shielding process. This new status of a virtual shortening of the gap results in a higher field emission from the cathode and could provide an important source of electrons, e.g. three times shorter cathode region equals three times larger electric field density in this layer.

Field emission [5] operates by providing a high electric field on the material surface, so that electrons are pulled of the surface by electrostatic forces. Electrons escape the metal via tunneling effect and the current density produced can be given by the simplified standard Fowler-Nordheim formula:

$$J_{FN} = \frac{A_{FN}\left(\beta_{FN}E\right)^2}{\Phi_w}\exp\left(-\frac{B_{FN}v(f)\Phi_w^{3/2}}{\beta_{FN}E}\right) \quad (7)$$

where Φ_w is the work function of the material in eV, $A_{FN}=1.541434\cdot10^{-6}AeV/V^2$, $B_{FN}=6.8308eV^{-3/2}Vnm^{-1}$ and $v(f)=1-f+(1/6)f\ln f...$, $f=1.439964eV^2V^{-1}nm\cdot E/\Phi_w^2$ take specific numerical values, while β_{FN} describes surface geometry effects, namely electric field enhancement. While a quick look does not reveal a significant current contribution, in reality appreciable currents are obtained at $\beta_{FN}E \sim 10^8 V/m$ - achievable if we take into account the significant β_{FN} due to microscopic protrusions that always exist in real metal surfaces. Field emission alone can result in the breakdown of vacuum gaps, but is highly dependent on the electrode material and surface.

3 PIC SIMULATIONS

Our simulation model is set up in a way, so that it would most resemble the experiment described in the beginning of the previous section. As it is presented in the Fig.2, the simulation setup consists of two opposing electrodes connected via external circuit. The distance between electrodes can be varied, as can the parameters of external circuit. The other part of the *pd product* can be changed via applying different number densities of the background gas. We would proceed in the following manner. A few electrons would be injected at the left electrode acting as a source cathode. Then the state would be saved into a dump file and high voltage would be applied between the electrodes and background gas pressure would be prescribed to the system. As electrons travel between the electrodes, avalanche processes fill the system with additional electrons and ions. Macroscopic as well as microscopic diagnostics is applied at an arbitrary moment to produce spatially and temporally dependant results like densities, temperature, etc. In our case the gas selected was Hydrogen since exact cross-sections for all particle-particle interactions were already available. The DC voltage applied between electrodes had been varied between -2500V and -25000V. Our goal was to study the effects of space-charge accumulation through observing the perturbation of the potential with the regards to the initial electron number injected – electron current.

Since this is a 1d code we would keep the initial number of electrons in the dump file intact, but rather change the area A of the simulation domain. In this way the current density $J_{initial}$ would be virtually increased, and perturbations would occur due to

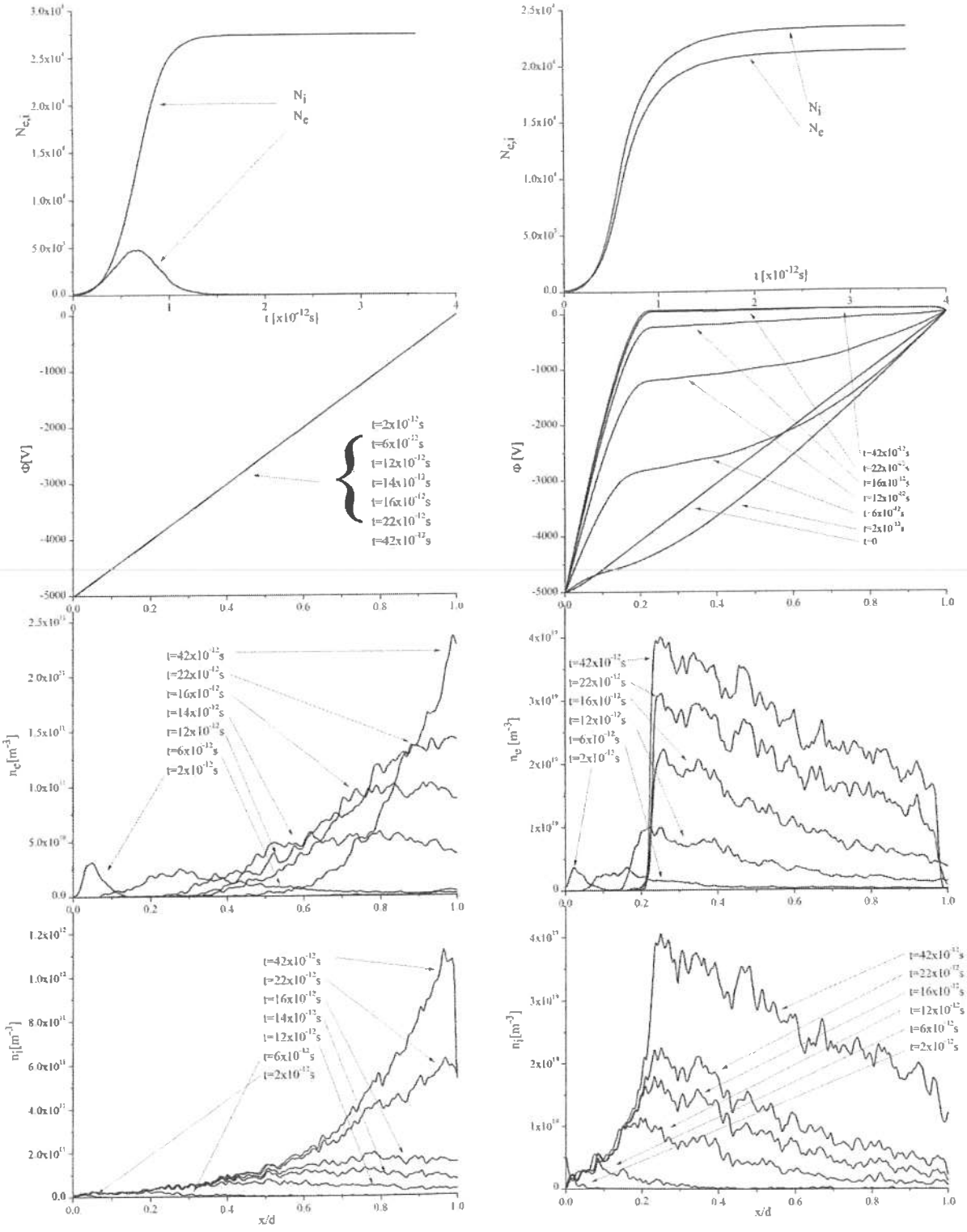

Figure 3: Number of electrons and ions in time (top), potential profiles, density profiles for electrons and ions at different times of avalanche process for two current densities $J_{initial}=4\cdot10^{-5}$ A/cm^2(top) and $J_{initial}=4\cdot10^{3}$

higher charge density, designated by the charge ρ divided by domain volume $A\cdot d$.

4 RESULTS AND DISSCUSION

In this section we will present some of the results that we have obtained through our method. Since PIC codes are essentially close to experimental work, there are always numerous basic conditions to consider when setting up such computational experiment.

Afterwards there often has to be a lot of "fine-tuning" done in order to get satisfactory results. Also in this case literally hundreds of simulations had to be run and tens of GBs of data were stored and evaluated to get what is expected- results that go along with theoretical postulates. Our goal was to investigate the space-charge build up in initial stages of the gas breakdown and its consequences on the discharge formation. All of work was done for single shot of 128 electrons at the left boundary electrode. Such large number was selected because of improved statistics instead of making more 1 electron single shots and averaging the data obtained.

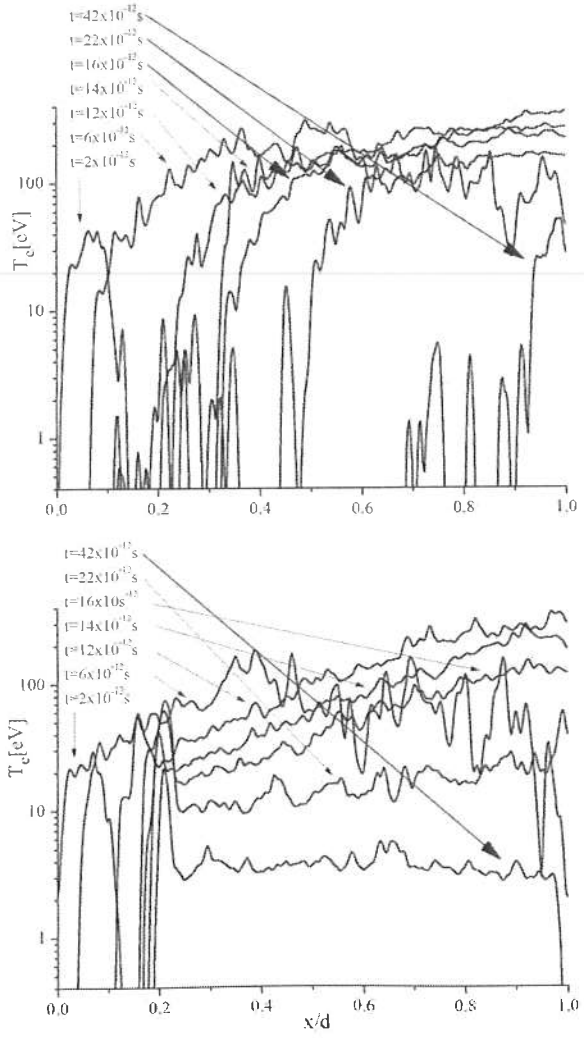

Figure 4: Temperature profiles at various times in avalanche phase at $J_{initial}=4\cdot10^{-5}$ A/cm^2(top) and $J_{initial}=4\cdot10^{3}$ A/cm^2(bottom)

Time steps, $dt=1\cdot10^{-15}$ s, used in the simulation had to be rather short, due to very fast particle movement. We shall focus our presentation on the case, where number density of the background gas (H_2) was $150\cdot10^{22}$ m^{-3} and the voltage between the two electrodes was V=5000 V. Electrodes were separated by a 1 mm gap, so *pd* product remained constant. In Fig. 3 we preset profiles of electron and ion densities and potential profiles in various moments of avalanche stage. Here we also present the number of electrons and ions in time during this phase. Following in the Fig. 4 are the time developments of particle temperature profiles shown. All this quantities are presented here for two extreme cases: a very small initial current density $J_{initial}=4\cdot10^{-5}$ A/cm^2 (left side) and for a large initial current density $J_{initial}=4\cdot10^{3}$ A/cm^2 (right side). Of course higher initial current density results in a higher particle density, even with roughly the same electron multiplication factor. Here we seek the formation of plasma, instead of just a low number of charged particles being produced, as plasma plays the role of the conductor in GDTs. Higher charged particle densities together with particle species temperatures are an important indicator of the transition between neutral ionized gases and plasmas. Plasma as quasi-neutral conducting media can shield itself from external perturbation with non-neutral regions called sheaths. The thickness of the shield can be estimated as being a few Debye lengths:

$$\lambda_D = \sqrt{\frac{\varepsilon_0 k T_e}{n_e e_0^2}}\,. \qquad (8)$$

That would mean that in order not to lose all the electrons immediately due to external electric field, the system has to be at least few tens of Debye lengths long to be able to form sheath. For low charged particle densities (order of 10^{-12}m^{-3}) and high temperatures (more than 100eV), as in the first case, Debye length would be much larger than the whole system. Since there is little interactions between charged particles, the electrons tend not to lose much energy in charged particle-charged particle interactions, and the temperature remains high. Ambipolar diffusion is negligible here. On the contrary, in the second case particle densities are much higher (order of 10^{-19}m^{-3}) and temperatures much lower (few eV). Ions draw energy from fast electrons in ambipolar flow, as strong electric fields in sheaths overcome the externally applied voltage, and microscopic fields dominate inside plasma. Debye length in this case is approx. $\lambda_D\approx2\mu$m, much less than the system length. Already from the particle number we can see the effect of higher particle density, as the electrons remain trapped inside the system for a longer period of time. Since ions are much heavier than electrons, they do not move much in the time period presented. This means, that the ion density profile is in a way a "footprint" of the ionization process. Profiles for the two cases are very different in a way, but both show the exponential increase from the beginning, according to avalanche formula (1). Since electric field *E* remains unperturbed in the first case, the profile as whole holds exponential "shape", while in second case the electric field is altered by the presence of high

charged particle density, so α has to be recalculated in (2) according to new value of electric field *E*. Therefore the whole process should rather be described in an integral form. The potential profile otherwise exerts sheaths on both sides, cathode and anode, so the potential in the middle is slightly positive. What can also be seen is, that for additional electrons injected in the domain with some delay, system would appear much shorter, only about 20% of the original length. Again the first Townsend coefficient would be unique for the oncoming particles. In addition to that, the electric field at the cathode would be approx. 5 times higher, which could significantly contribute to higher field-enhanced emission according to (7).

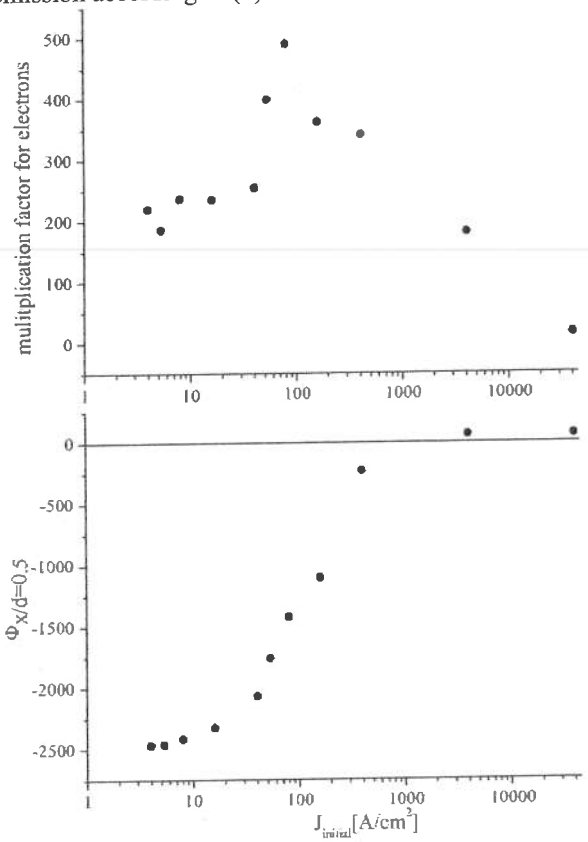

Figure 5: Electron multiplication factor (top) and potential Φ(x/d=0.5) for various $J_{initial}$

In the top of Fig. 5 we present the values of the electron multiplication factor for various initial current densities $J_{initial}$. The profile shows a distinct peak in the mid-range, and also a tendency towards zero for very high initial current densities. The latter can be explained with high density plasma (formed soon after the first shot of particles) slowing down most of the electrons to below the ionization energy. In the bottom graph we present the dependence of the potential of a point placed at x/d=0.5 on the initial current density $J_{initial}$. We can see how space-charge starts affecting the potential profile around $J_{initial}$=10A/cm^2 for this set of parameters - a realistic value for GDT use. Therefore, space-charge effects should be further examined.All in all, from an engineering point of view we can draw some conclusions. Parameters, such as *pd product*, expected over-voltage pulse, have to be taken into account when constructing GDTs, so as to make the most use of space-charge effects. This could be especially useful for production of successive shots of electrons from the cathode via increased field emission. Material processing should also play an important role here, as perhaps a cathode with microscopic spikes could further enhance field emission.To conclude, PIC codes have proved to be a useful tool for gas breakdown studies, but many physical processes, like field emission, still need to be implemented to be able to simulate the whole breakdown.

Acknowledgments

This work is supported by Slovenian Ministry of Science and Technology by grant No L2-3652 "Raziskava in razvoj integriranih prenapetostnih zascitnih naprav na osnovi plinskega odvodnika (GDT) v smeri zanesljive miniaturizirane tehnicne resitve (MINIGDT)". Simulations were performed at new University supercomputer Prelog which is installed on FS.

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