Ignition Process of Microplasmas

H. E. Porteanu[*1], R. Gesche[1]
[1]Ferdinand-Braun-Institut für Höchstfrequenztechnik
*Corresponding author: Gustav-Kirchhoff-Str. 4 12489 Berlin, porteanu@fbh-berlin.de

Abstract: Microplasmas at atmospheric pressure are required in many applications, where treatments in normal ambient, with spatial resolution, are important. The interest on such miniaturized sources has increased due to the availability of a new generation of microwave sources based on high power GaN transistors. The present work deals with a simulation of the plasma formation after the application of the microwave power. The results are needed for the optimization of the GaN oscillator, directly coupled to the plasma source. The slot resonator used in experiment is simulated by a 2D geometry representing two spatially, infinitely extended, parallel metallic plates. The self consistent calculations are performed using COMSOL multiphysics.

Keywords: nitrogen plasma, microwave plasma generation, atmospheric pressure, coupled differential equations.

1. Introduction

The generation of stable plasmas can be easily done using microwave generators. A large number of chemical processes make use of such plasma sources. The standard configuration consists of a low pressure chamber, in which are placed the objects to be processed. Depending on the chemical reaction, different gases at pressures of about 1 mbar fill the chamber and are maintained in plasma state using strong RF fields. This arrangement is very useful for industrial processes, but less for medical or biological applications. Even in industry there are situations, where a local cleaning, etching, or surface activation in simple conditions, at atmospheric pressure, is required. Moreover, the tendency in the lightening industry is to use high pressure, miniaturized lamps, driven by microwaves. The plasma display industry uses microplasma sources that have to be not only very efficient but their ignition and extinction have to be very well controlled. In all these situations is required an adequate modeling of the interaction of the RF electromagnetic field with the plasma.

An example of plasma source is the quarter-wavelength slot resonator. Fig. 1 shows a picture of the working resonator at 2.3 GHz and the COMSOL model.

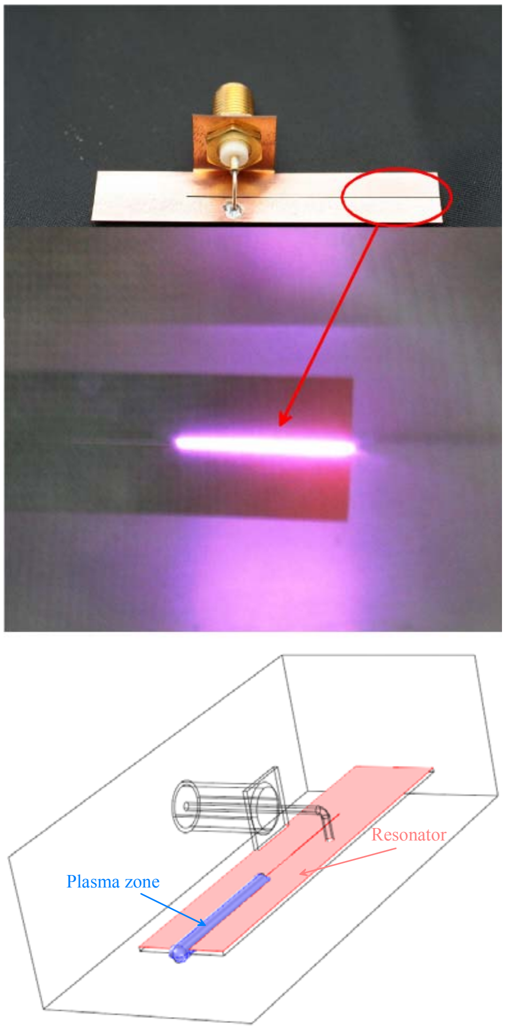

Figure 1. Top: the quarter-wavelength slot resonator is made of a copper plate, 0.2 mm thick and has a 3.75 cm long and 0.1 mm broad slot. Plasma appears as a quasi-homogeneous discharge over ~2 cm length. Bottom: 3D model used in COMSOL

2. Theoretical Approach

The resonator presented in Fig. 1 is a precursor for further applications and a good tool to examine plasma in simple conditions. With the 3D geometry presented in Fig. 1 we can calculate the reflection coefficient (or generally the complex S_{11} parameter) using the RF module of COMSOL. The simple implementation of the Maxwell equations gives information about the bulk field and surface current distributions. The blue marked zone, where plasma appears, was defined in COMSOL as a medium with a homogeneously distributed and predefined conductivity that fits our experimental results. A detailed investigation of the plasma equivalent impedance and effective complex conductivity is presented in ref. 1.

The complexity of this 3D geometry does not allow in present a detailed self consistent computation of the plasma evolution. Therefore, we made a rough approximation by considering a parallel plate resonator with the distance between plates being equal to the slot width (0.1 mm). In our experiment there is a gas flow of ca. 1 cm^3/s that is in our estimation much smaller than the electron thermal speed. Adjustment of this gas flow in limited range does not change considerably the plasma behavior. Therefore we neglect in the present implementation this contribution.

2.1 RF Module

We consider in this model that the wave propagates in x direction (horizontal), the electric field is oriented in the x-y plane and the magnetic field in the z direction. The corresponding wave equation for the TM mode is:

$$\nabla \times \left(\left(\varepsilon_r - \frac{j\sigma}{\omega\varepsilon_0} \right)^{-1} \nabla \times H_z \right) - \mu_r k_0^2 H_z = 0$$

The microwave field oscillates with the frequency ω. The period is much shorter than the thermal and diffusion processes in plasma. Therefore, at this stage there is a simple harmonic variation and the time derivative is replaced by multiplication with $j\omega$ ($j=\sqrt{-1}$). The dielectric and magnetic permittivity (ε_r and μ_r) are equal to 1. The complex conductivity σ depends on the electron concentration and the scattering rate ν.

$$\sigma = \omega_p^2\, \varepsilon_0 \frac{1}{\nu + j\omega}$$

here ω_p is the plasma frequency,

$$\omega_p^2 = \frac{ne^2}{m\varepsilon_0}$$

We consider simplified only the contribution of electrons to conductivity. The scattering rate is an effective value obtained by averaging all types of collisions over the entire range of electron energies. We use a statistical description of the form:

$$\nu \propto T_e^{3/2} N,$$

where T_e is the electron temperature and N is the density of neutral molecules of nitrogen (e.g. N=2.687 10^{19} cm^{-3} for T=300 K and p=1 bar). This estimation for ν is an approximation that has to be refined in the future.

2.2 Plasma fluid equations

We follow the standard notation in the plasma physics, by multiplying the temperature with the Boltzmann constant (k_B=1.3806 10^{-23} J/K). Therefore the gas law appears simply $p=NT$ (p is the pressure, N the molecular density and T is the *internal energy* expressed in J or eV).

In order to solve the RF module, the medium conductivity has to be defined; therefore two input magnitudes are necessary: the electron density n and their scattering rate ν as function of position **r**. They are determined with the following modules: (1) diffusion and convection and (2) general heat transfer.

The general plasma kinetic theory is based on the Boltzmann equation, using the (unknown) distribution function $f(x,v,t)$. The zero order momentum represents the particle conservation equation. The first order momentum of the distribution function yields the momentum conservation, whereas the second order the energy conservation. In the present context we describe the fluid motion with help of space dependent, average magnitudes as the electron density or the temperature (equivalent to the electron kinetic energy).

The continuity equation for electrons requires that:

$$\frac{\partial n}{\partial t} + \nabla\Gamma = G - R,$$

Γ is the electron flux, G is the ionization rate (in the same time the generation rate for electrons), and R is the recombination rate. The total charge of the system is zero. Therefore the corresponding continuity equation for ions gives the same total (integrated) charge as function of time. The generation and recombination rates, G and R are the same for ions. There are many reactions as result of collisions between free electrons and N_2 molecules or ions. An example of them is listed in ref. 2. Numerical data calculated for the reactions listed in ref. 2 are in given ref. 3. For the sake of simplicity we present here an empirical model, originating from Towsend. The ionization rate G is expressed as G=α v_D. The ionization per unit length α has the form: $\alpha = Ape^{-Bp/E}$. For nitrogen A=12 $cm^{-1}Torr^{-1}$, B=342 V/(cmTorr), E/p=100-600 V/(cmTorr) and p is the pressure, $p=nT_{gas}$ [4]. The diffusion velocity v_D is in this context close to the thermal velocity of electrons, $v_D = \sqrt{\frac{2T_e}{m_e}}$. The recombination rate is $R = \frac{n_{e0}}{1+n_{e0}\beta t} \sim \frac{1}{\beta t}$. According to ref. [4] the coefficient β for nitrogen is of the order 10^{-7} cm^3/s.

The electron flux Γ is obtained from the momentum conservation on a long time scale. The quick motion, synchronous with the microwave driving field, is averaged (i.e. zero) in the following expression. The quick dynamics appears in the expression of the complex conductivity σ. Therefore,

$$\Gamma = -\frac{\nabla p}{m_e \nu} = -\frac{\nabla(\mathrm{nT_e})}{m_e \nu} = -\frac{\mathrm{T_e \nabla n + n \nabla T_e}}{m_e \nu}$$

The expression for Γ together with the electron continuity equation was implemented in the module "Convection and Diffusion". For a given electron temperature, generation and recombination rates, the module yields the electron density $n(\mathbf{r},t)$. The ion diffusion and the resulting ambipolar electric field are not yet implemented.

The energy conservation uses formulations defined in refs. 5 and 6. Our simplified formulation neglects the ion motion and the viscosity tensor (π=0). The unique energy source is the joule heating, i.e. $W_e = Re\{\sigma\}|E|^2$. The energy dissipated by collision with ions is included in W_e, therefore:

$$\frac{3}{2}\frac{\partial(nT_e)}{\partial t} + \nabla Q_e = W_e$$

The energy flux Q_e is related to the particle flux Γ with the following formula:

$$Q_e = \frac{5}{2}T_e\Gamma - \lambda \nabla T_e,$$

where the electron thermal conductivity λ is

$$\lambda \sim \frac{5}{2}\frac{nT_e}{m_e \nu}$$

Because the electron flux results from a temperature gradient only (the gas flow is absent), the energy flux contribution due to thermal conductivity is comparable, in our simulation is considered as equal to the first term. The "Heat Transfer by Conduction" module treats only the temperature variation for solids, where n is constant. We used this module by changing the variable $p_e=nT_e$. For a given n and electric field E, this module yields the product nT_e, or, indirectly, the electron temperature T_e. The electron temperature determines the scattering rate ν. In this way the electromagnetic wave module is completely determined.

2.3 Boundary conditions

The module "Convection and Diffusion" uses the condition (electron) "Flux" set to zero. The module "Heat Transfer by Conduction" uses the condition "Heat Flux" to outer temperature (T=300 K) using a heat transfer coefficient specific for air (~10 W/m^2K).

3. Simulation results

The investigation of the ignition process requires not only equations and boundary conditions, but also a certain initial state. The initial electron density is not zero. According to [4] there is always a residual density of electrons of the order 10^3 cm^{-3}. This amount is enough to get hot in the microwave field and to ionize additional atoms or molecules. Experimental details about the ignition process studied on the slot resonator are presented in ref. 7 and 8.

Fig. 2 presents the evolution during the first 10 µs of the magnetic field H_z.

The propagation takes place from left to the right. The magnetic field is perpendicularly oriented to the paper plane.

We have chosen only for computational and illustration reasons a much higher frequency in order to evidence the variation of the instantaneous microwave field intensity.

Fig. 3 shows the electric field component E_x at the beginning and at the end of the ignition

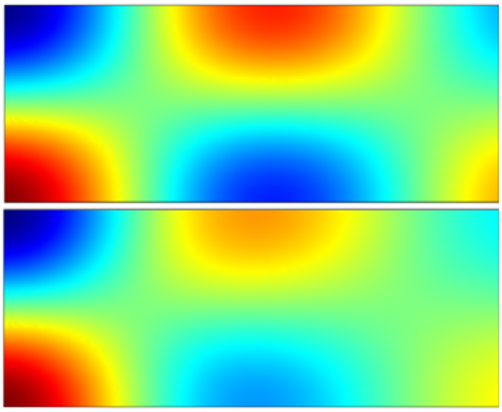

Figure 2. Top: The magnetic field distribution (instantaneous values) before ignition of plasma. For illustration purposes we have chosen a greater distance than lambda-quarter. Bottom: the same distribution after the ignition.(red, $H_{z,max}$, blue, $H_{z,min}$)

process. Such a longitudinal component is not zero because the potential of the both planes is set to zero. This distribution is typical for a waveguide propagation but also for the actual structure of the resonator, which is embedded in a metallic case.

The evolution of the free electron density is presented in Fig. 4. The heating of the electron gas leads to an increase of the temperature that has as consequence a higher ionization rate and increase of the electron density. However, in the regions with high electron density the conductivity is high and the electromagnetic

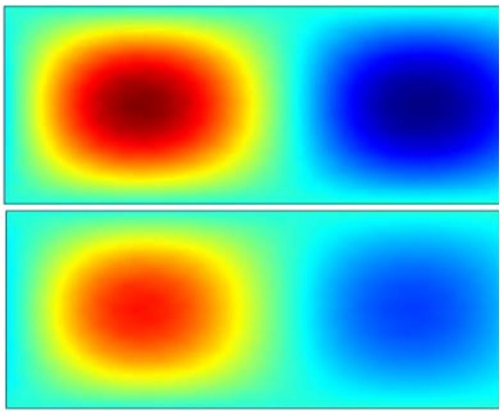

Figure 3. Top: the longitudinal electric field E_x distribution (instantaneous values) before the ignition of plasma. Bottom: the same distribution in the steady state regime.

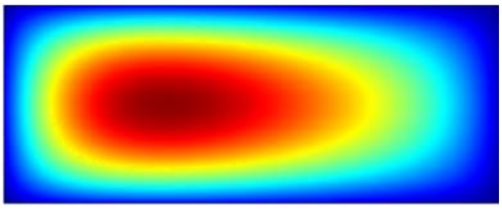

Figure 4. The electron concentration after plasma has stabilized. Initially there is a homogeneous distribution of residual free electrons of about 10^3 cm^{-3}, [4].

field is partially absorbed and partially reflected. Additionally, the electrons diffuse from the generation zone with high temperature.

The heating process appears in Fig. 5. The hot spot is more localized than the electron density because of a slower energy diffusion than electron diffusion (ions store energy as well). The metallic walls absorb a part of the energy.

The competition between heating, electron generation, screening and again cooling is in general very complex. It is better visible in the time dependence of the reflection coefficient ($|S_{11}|^2$ (dB)), as presented in Fig. 6.

7. Conclusions

We present our first successful implementation of a plasma simulation, using the COMSOL program with coupled differential equations in a transient regime.

8. References

1. H. E. Porteanu, S. Kühn, and R. Gesche, Low Power Microwave Plasma Conductivity,

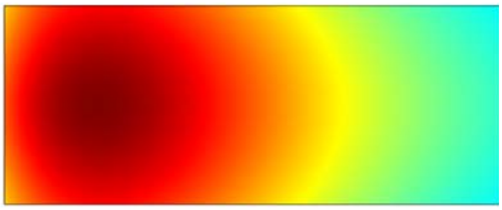

Figure 5. The electron temperature in steady state regime. The initial temperature was 300 K

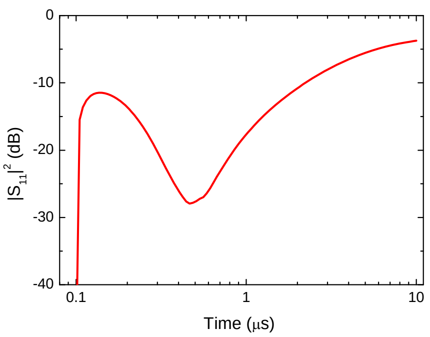

Figure 6. Time evolution of the reflection coefficient expressed as $|S_{11}|^2$. The values close to 0 dB evidence the screening effect of the free electrons.

accepted for publication at *IEEE Transactions on Plasma Science.*

2. E. Tatarova, F. M. Dias, C. M. Ferreira, V. Guerra, J. Loureiro, E. Stoykova, I. Ghanashev, and I. Zhelyazkov, *J. Phys. D: Appl. Phys.* **30**, 2663 (1997).
3. A. V. Phelps and I. C. Pitchford, *JILA Information Center Report* (Boulder, CO: Colorado University) No. 26 (1985).
4. Y. P. Raizer, *Gas Discharge Physics*, Springer (1991).
5. R. Fitzpatrick, *Introduction to Plasma Physics*, Lulu (2008).
6. M. A. Lieberman, A. J. Lichtenberg, *Principles of Plasma Discharges and Material Processing*, Wiley (1994).
7. H. E. Porteanu, S. Kühn, and R. Gesche, Ignition delay for atmospheric pressure microplasmas, submitted to *Contributions to plasma physics.*
8. S. Kühn, H. E. Porteanu, and R. Gesche, Plasma impedance dynamics during the ignition process, to be published.