Numerical investigation of the effect of insulator permittivity on the initial stage of dielectric barrier discharge

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Abstract. We present a numerical simulation of the simplified ferroelectric plasma source operating in a gas discharge mode. The plasma source contains two electrodes separated by a ferroelectric. High voltage pulse applied to the cathode leads to formation of a dielectric barrier discharge in gas (argon at 1 Torr pressure). The main point of the study is to clarify how the high permittivity of the ferroelectric affects the initial stage of the discharge. Two cases are considered with different values of barrier relative permittivity. The results show that the process of compensation of bound charge affects the electron avalanche formation near the dielectric surface. The electron concentration in the avalanche drops down for materials with higher permittivity.

1. Introduction
Ferroelectric plasma cathodes are widely used in particle accelerators [1-2]. Some other applications are active flow control [3] or aerospace thrusters [4]. They are known to provide high electron currents while being simple and compact devices. Two modes of operation of such devices are possible: vacuum, when the mean free path of electrons is greater than the distance between the electrodes [1, 2, 5, 6], and gas mode [3, 7], when the mean free path is small compared to this distance. The role of ferroelectric in the gas discharge mode has not been well understood to date. Due to the high speed of the ongoing processes, numerical simulation is a convenient tool for studying dynamics of the discharge.

In the vacuum mode a triple junction point between ferroelectric cathode and vacuum after applying the driving pulse becomes the source of electrons through field emission process. The high permittivity of the ferroelectric is beneficial in that case because it helps in creating a high tangential component of the electric field that accelerates the electrons. The surface discharge along the ferroelectric leads to a secondary emission of the electrons and a significant degassing of the material of ferroelectric into the vacuum. During this degassing the pressure may rise to levels where the discharge may switch to a gas mode. For the cathodes of several-centimeter scale the pressures ~1-10 Torr should be enough for the mean free path to drop to ~10^-5m. For such pressures the electron avalanches in the gas will start affecting the discharge process, lowering the electrons energy and, thus, reducing the secondary emission from the ferroelectric surface. With growing pressure the role of gas processes becomes dominant thus switching the mode of the discharge.

After switching to a gas mode the process becomes similar to an ordinary dielectric barrier discharge. However, high permittivity of the ferroelectric may still play some role in the discharge process because of the high amount of bounded charge that appears at the dielectric surface. The
process of dynamic compensations of these bound charges, especially at low electron concentration in the plasma may affect significantly the initial stage of the discharge. Strong depolarization fields that arise in the process of polarization switching of the ferroelectric allow lowering the operational voltage [3]. This is another distinct feature of the ferroelectric barrier discharges.

It is interesting to see how the high permittivity of the ferroelectric will affect the gas discharge under moderate pressure conditions compared to a low permittivity dielectric.

In the current paper we consider numerical simulation of a simplified case of a dielectric barrier discharge in argon at 1 Torr pressure. Two cases with high ($\varepsilon_r=2000$) and low ($\varepsilon_r=2$) relative permittivity are considered. The effects of domain walls motion in the ferroelectric are omitted in the current simulations for simplicity.

2. Computational methodology

To simulate dielectric barrier discharge in gas, we used a custom 2D finite-difference PDE solver for continuous media. The code utilized second order compact schemes for spatial discretization on a staggered grid. The electric potential was calculated at the grid cell centers while the species concentrations were calculated at the grid nodes. For time discretization second order implicit Crank-Nicolson scheme was used. The electron impact reactions rates were calculated by iterations of Newton’s method.

The simulations were done on a 2D Cartesian grid with immersed boundary method for setting up the electrodes’ surfaces.

The program includes the coupled solution of evolutionary equations in a drift-diffusion approximation:

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \Gamma_e = R_e$$ (1)

$$\Gamma_e = -\left( \mu_e \tilde{E} \right) n_e - \nabla \left( D_e n_e \right)$$ (2)

equation (1) for concentration of electrons $n_e$, where $R_e$ is the ionization rate from impact reactions and $\Gamma_e$ is electron flux (2) where $\mu_e$ and $D_e$ are the electron mobility and diffusivity coefficients;

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot \Gamma_{\varepsilon} + \tilde{E} \cdot \Gamma_e = R_e$$ (3)

$$\Gamma_{\varepsilon} = -\left( \mu_{\varepsilon} \tilde{E} \right) \varepsilon - \nabla \left( D_e \varepsilon \right)$$ (4)

equation (3) for electrons kinetic energy density $\varepsilon$, where $R_e$ is the impact reactions energy gain/loss and $\Gamma_e$ is the flux term (4).

$$\rho \frac{\partial \omega_k}{\partial t} + \nabla \cdot \left( \rho \omega_k z_k \mu_k \tilde{E} - \rho D_k \nabla \omega_k \right) = R_k$$ (5)

Evolution equation (5) for heavy species mass concentration ($\omega_k$) was solved for two species: positive argon ions (Ar$^+$) and metastable argon (Ar$^*$). Here $\mu$ denotes mobility of the specie; $D$ is the diffusivity, $\rho$ is the mixture density, $z_k$ is the charge of k-th specie. The source terms $R$ were calculated from electron impact reactions assuming Maxwell distribution of the electron velocities.

$$\nabla \cdot \left( \varepsilon \tilde{E} \right) = \rho_q$$ (6)

The electric potential was calculated by solving the Poisson equation (6) assuming electrostatic approximation ($\varepsilon$ – permittivity, $\rho_q$ – charge concentration).

At the cathode, secondary emission was modeled with the emission coefficient of 0.25. As we were interested in the initial stage of the discharge which had short timescale the heavy species were considered isothermal (at the temperature of 300K).
The thermodynamic parameters of the gas and the collision cross-sections of several electron impact reactions for argon were used (cross-sections data was taken from the open database LXCat www.fr.lxcat.net).

The set of used reactions is presented in Table 1.

| Reaction               | Type                  | $\Delta E$ (eV) |
|------------------------|-----------------------|-----------------|
| $e + Ar \rightarrow e + Ar$ | Elastic collision     | 0               |
| $e + Ar \rightarrow e + Ar^*$ | Ground state excitation | 11.5           |
| $e + Ar^* \rightarrow e + Ar$ | Superelastic collision | -11.5          |
| $e + Ar \rightarrow 2e + Ar^*$ | Ground state ionization | 15.8           |
| $e + Ar^* \rightarrow 2e + Ar^*$ | Stepwise ionization   | 4.24            |

**Figure 1.** Schematic view of the simulation domain.

The simulation domain is shown in Fig.1. The simulated setup consisted of anode, cathode and insulator. The insulator was a flat plate with a length of 20 mm and a width of 1 mm. Above the insulator the cathode of 0.5 mm width and 2 mm length was located. The anode was located below the insulator at its whole length except for the part just below the cathode. Such setup was chosen to maximize the tangential component of the electric field.

Argon atmosphere of 1 Torr pressure and 300K temperature was assumed. Initial electron concentration was chosen to be $10^{13}$ m$^{-3}$. To start the discharge a negative voltage was applied to the cathode in the form of a short stepwise pulse with 400 V magnitude. The numerical grid consisted of 500x250 grid points with the refinement towards the cathode and insulator surfaces (the smallest grid step size at the wall was 0.01 mm). The timestep was $10^{-11}$ s. The total simulation time was 100 ns. After that time a cathode sheath was formed. We considered two cases with different values of relative permittivity: cases A and B (with permittivity of 2 and 2000, respectively).

3. Results and discussion

After the initial voltage pulse the discharge starts from the triple junction point at the cathode. Near this point the field gets amplified because of the sharp corner of the cathode. For the case B the tangential component of the field becomes even more intensified by the high permittivity of the ferroelectric. The peak tangential field strength is $10^6$ V/m in case A and $4.5 \cdot 10^6$ V/m in case B, while the mean field magnitude in the discharge region is $\sim 10^5$ V/m. This shows a significant field intensification effect. However, the impact ionization in the gas leads to a fast compensation of the bound charge at the ferroelectric surface thus reducing the field strength significantly near the triple junction.

The process of the dielectric charging leads to the formation of a fast moving electron cloud (Fig. 2). The electron cloud detaches from the cathode and rapidly moves along the ferroelectric with
velocities of the order of $10^6$-$10^7$ cm/s. Similar speeds are reported for the plasma front propagation in some ferroelectric plasma cathode experiments [2]. While moving away, the electrons from the cloud compensate the bound charges on the dielectric surface. As the cloud moves away from the cathode, the tangential component of the field weakens and the motion of the cloud slows down. After ~10 ns the cloud of electrons begins to detach from the surface of the dielectric. The travel distance of the cloud is ~10-12 mm in both cases. After about 100 ns the anode field becomes screened by the attached electrons leading to the formation of cathode sheath (Fig 2, bottom).

**Figure 2.** Electron concentration distribution (m$^{-3}$) at different time instants of the discharge. Left column: $\varepsilon_r =2$ (case A). Right column: $\varepsilon_r =2000$ (case B).

The main difference between cases A and B is that the number density of electrons is about 1.5-2 times weaker for the case with high permittivity because more electrons should attach to the surface to compensate for the bound charge in that case. In this case, the process of compensating bound charges is slower and requires more charge, which leads to a change in the shape of moving cloud of electrons and a decrease in the concentration of particles in it, compared with the case of a small dielectric constant.
The positive ion distribution (Fig. 3) has a shape similar to the electron distribution at the beginning of the discharge, but after the initial cloud formation the ions do not travel with the electrons but stay attached to the cathode. It is interesting to note that the ion distribution attaches to the upper angle of the cathode thus indicating that the field at the triple junction point (which was the highest at the beginning of the discharge) becomes compensated by the attached electrons. Comparing the cases A and B it can be seen that, similar to the electrons distribution, the ions in case B also have smaller concentrations than in case A. This should reflect a lower electron flux values in this case which is connected to the loss of electrons to the insulator charging.

Figure 3. Positive ions (Ar+) concentration distribution (m$^{-3}$) at different time instants of the discharge (a, c) – 5 ns; (b, d) – 15 ns. Left column: $\varepsilon_r$ = 2 (case A). Right column: $\varepsilon_r$ = 2000 (case B).

Conclusions
We have simulated the dielectric barrier discharge in argon over the insulators with high and low permittivity for moderate pressure conditions (1 Torr). The effect of the permittivity on the initial stage of the discharge has been studied.

Because of the impact of ionization processes in gas the higher horizontal electric field magnitude in case of high permittivity insulator does not lead to a significant intensification of the discharge intensity. The collisions in the gas do not allow the electrons to reach sufficiently high energies; and the effect of initial field amplification by the ferroelectric only leads to the emergence of more electrons near the triple junction point. These excess electrons then very rapidly compensate the bound charges at the surface of ferroelectric, diminishing the field amplification effect. However, high permittivity of the insulator affects the initial stage of the discharge when a cloud of electrons is moving along the insulator surface. Higher amount of bound charge in this case leads to a weaker electron cloud as more electrons are spent on the compensation of the bound charges. These effects require additional investigation in the transient regime between the vacuum and gas modes of the discharge. The effect of polarization switching on the gas discharge should also be considered in the future work.

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