Numerical simulation of domain wall motion in a surface discharge over a ferroelectric

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Abstract. The article presents a simplified numerical simulation of a vacuum ferroelectric cathode operating in a low-current mode (without surface plasma formation). The field emission from the cathode was simulated for the range of applied electric field magnitudes. The polarization domain growth process during the charging of ferroelectric surface was simulated using Landau-Ginzburg-Devonshire model. Interaction of the electrons with a depolarization field of a domain wall led to an attraction of the electrons to the polarization domain boundaries. A close to the linear dependence of the equilibrium domain wall position from the applied electric field was found with the total emitted charge proportional to the domain size.

1. Introduction
An electric discharge over a ferroelectric has several interesting properties associated with the domain structure in the material, as well as with a large value of surface charges and depolarization fields between neighboring domains. These properties of ferroelectrics find their application in particle accelerator technology, where ferroelectric cathodes are used as inexpensive and compact sources of electron beams [1,2].

At the same time, the complex dynamics of the discharge under these conditions is difficult to study directly in the experiment due to the high speed of the ongoing processes, as well as their strong nonequilibrium behavior. For that matter, a numerical simulation can provide some useful information about the discharge process. Usually, the simulations of this kind are limited to only electric field calculation using the Poisson equation, sometimes coupled with the simplified approximation for the polarization distribution in the ferroelectric [3]. For the surface discharge over a normal dielectric, the full simulation with Lagrangian (Particle-in-Cell, “PIC”) approach for electrons [4] is usually done. However, for the ferroelectric, it is essential to simulate the polarization dynamics because the domain walls act as a source of strong depolarization fields [3] and the switching process may affect the field emission process and the dynamics of the discharge.

In the current paper, a 2D idealized simulation taking into account both the electrons and polarization dynamics was considered. In this work, we investigated the vacuum (field-emission) discharge mode with an asymmetric arrangement of electrodes in a two-dimensional formulation (Fig. 1). The fully Lagrangian approach was considered which allowed for an accurate reconstruction of electric fields at the cathode surface.
2. **Computational methodology**

The upper electrode (cathode) had a prismatic shape with a height of 50 μm and a 60 degrees angle of the side plane with the ferroelectric film (Fig. 1). The lower electrode (anode) was an extended flat plate. A 50 μm thick ferroelectric film was placed between the upper and lower electrodes. The length of the film was 0.5 mm. The computational domain had dimensions of 0.8 × 0.8 mm. The vacuum conditions were assumed with a mean free patch of electrons larger than the domain size.

![Figure 1. The scheme of the computational domain. The color of the film shows the direction of the polarization vector (red – up, green – down). The applied voltage between the electrodes is 500 V and the shown time moment is 10 ns after the discharge starts.](image)

To calculate the electric field, a grid-free solver was used for the Poisson equation using an approach based on Green's function solutions superposition [5]. The electrodes were discretized by surface potential monitoring points and fictitious field sources that were placed inside the electrodes at the distance equal to the local step between neighboring monitoring points. The electric potential was assumed as a superposition of the sources from these fictitious charges, free charges of the electrons, and the bound charges at the surface of ferroelectric (1).

\[
\varphi(\vec{r}) = -\frac{1}{2\pi \varepsilon_0 h} \sum q_i \ln(|\vec{r} - \vec{r}_i|); \quad E = -\nabla \varphi
\]  

(1)

where the summation is assumed over all charges in the system, \( h \) is the computational domain size in \( z \) (off-plane) direction (50 μm in the current simulation).

At the electrodes, the fixed potential conditions were set thus leading to a system of linear equations for the values of the fictitious charges. The equations were solved by a Gauss elimination method. The described method allows finding solutions for an arbitrary shape of electrodes and can be easily expanded to three dimensions.

The ferroelectric was considered in a simplified formulation, for the regime of 180-degree domains with one polarization component, normal to the film surface, whose dynamics was resolved according to the Ginzburg-Landau-Devonshire model [6] (2), while the properties of the ferroelectric were taken similar to those of BaTiO\(_3\).

\[
\frac{\partial P_i}{\partial t} = E - 2\alpha_0 (T - T_0) P_i + 4\beta P_i^3 - 6\gamma P_i^5
\]  

(2)

The parameters were chosen to be appropriate for a BaTiO\(_3\) single crystal, \( \alpha_0 = 3.34 \times 10^5 \) Vm/C, \( T_0 = 381 \) K, \( \beta = 6.38 \times 10^8 \) Vm\(^3\) C\(^{-1}\), \( \gamma = 7.89 \times 10^9 \) Vm\(^9\) C\(^{-5}\).

The polarization was assumed to be uniform over the thickness of the ferroelectric, so the discretization was done only in the longitudinal direction by small rectangular elements (of a few-nanometer size). The equation (2) was solved by iterations of Newton's method. The influence of polarization on the remaining elements of the system was done through the introduction of point charges distributed on the surface of the ferroelectric, and corresponding to the magnitude to the bound charges, which were proportional to the polarization of the element.
The free electrons were represented by particles (parcels), each containing the charge of 100 $e$ (elementary charge). The electron dynamics in free space was solved by time-integrating the Lagrangian trajectories of the particle (3)

$$\frac{dv_e}{dt} = -\frac{e}{m_e} E(x, y)$$

Upon hitting the surface, the electrons’ charge partially compensated the bound charge, which led to the screening process. Field emission from the electrode surface was calculated according to the Fowler-Nordheim law [4] from the place of maximum field concentration (4)

$$J(E) = \frac{1.54 \times 10^{-6} \beta^2 E^2}{1.1 \phi} \exp \left( \frac{-6.83 \times 10^7 \beta^{3/2} \theta(y)}{\beta E} \right)$$

$$y = 3.79 \times 10^{-4} \sqrt{\beta E / \phi}$$

$$\theta(y) \approx 0.95 - 1.03 y^2$$

where $\phi$ (in eV) is the work function of the cathode material (4.7 eV), $E$ is the electric field in V/cm, and $\beta_2$ is the electric field enhancement factor (set equal to 100 in the current paper).

Secondary emission of electrons could occur from the surface of the ferroelectric if the local sign of the vertical electric field component in this place changed and the field could no longer hold the attached electrons.

3. Results and discussion

![Figure 2](image)

**Figure 2.** Evolution of attached charge at the ferroelectric surface (a), domain wall coordinate (b), the ratio of surface charge to domain wall position at the moment of transition between “fast” and “slow” stages of the discharge (c), domain wall coordinate (at the moment of transition) vs applied voltage (d).
The simulation starts from the totally switched conditions of the ferroelectric, with a bound charge compensated by the attached charge (assuming a long exposure to the reversed electric field). Then the voltage is applied to the electrodes and the discharge process starts. When the polarization domain starts forming, a large depolarization field appears at the domain wall. This field has a strong horizontal component and when the wall is close to the metal-ferroelectric-vacuum triple point it promotes the field electron emission from the electrode.

Subcritical regimes of the discharge were considered, without forming a secondary electron avalanche. During the discharge, electrons fell onto the ferroelectric, which led to its switching and domain growth from the metal-ferroelectric-vacuum triple point. The attached charge was accumulated on the surface above the domain. In the process of domain growth, gradual screening of the external field occurred, which reduced the emission current and led to the rapid slowing down of the domain wall at a certain distance from the triple point. As the domain grows the electrons that hit the ferroelectric behind the domain wall start to screen the electric field, and the point of maximum emission on the cathode is shifted upwards. Due to the interaction with the depolarization field at the domain wall, the newly emitted electrons tend to hit the ferroelectric in front of the domain wall thus promoting the domain growth. When the screening effect reduces the electric field at the cathode significantly, the emission process slows down and the domain wall motion becomes slower than the accumulation of the charge at the surface of ferroelectric. This is noticeable in comparison to Fig 2a and Fig 2b depicting the accumulated charge and the domain wall position during the discharge process.

The graphical dependence of the domain wall position on time for different applied voltages is shown in Fig. 2b. It can be seen that the discharge has a fast first stage associated with polarization switching and a slow second stage when the residual field is screened by electrons. The transition between these two stages occurs at some critical equilibrium position of the domain wall. It can be seen that the equilibrium position of the wall is almost linearly dependent on the voltage (Fig. 3d). The charge accumulated before the transition is proportional to the domain size (Fig. 3c).

The distribution of charge at the surface of ferroelectric after the transition is shown in Fig. 1. At the surface of ferroelectric, the attached charge is concentrated mostly above the ferroelectric domain with some gradual decrease from the triple point toward the end of ferroelectric. This decrease reflects the screening of external electric field by electrons. The accumulated charge surface density is close to the spontaneous polarization of the ferroelectric (0.26 C/m²). At the late stages of the discharge, some secondary domains start growing close to the domain boundary (Fig. 1). These secondary domains are formed to balance the weakened external electric field and the depolarization fields at the domain boundaries.

4. Conclusion
The barrier discharge in a vacuum over the ferroelectric film was simulated, and the effect of the polarization domain growth during this process was studied.

The high permittivity of ferroelectric allows accumulating a significant amount of screening charge at the surface of the film which is compensated by a bound charge. The charge accumulation is accompanied by the effect of polarization switching and the domain wall motion. The depolarization field which is formed at the domain wall affects the distribution of free electrodes at the film surface. Most of the electrons are contained above the switched area. The discharge has two distinct stages, one fast which is attributed to the domain growth, and the other slower, attributed to the screening of the external electric field with more diffusive switching of the ferroelectric. The domain size at the moment of transition was found to depend almost linearly on the applied voltage.

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