REASON FOR FREE ELECTRONS FROM THE SURFACE OF FERROELECTRICS WITH A METAL LATTICE STRUCTURE

H. Heydari[1], T. Tille[1,2]

[1]Institute of Theoretical Electrical Engineering, Technical University of Berlin, Germany

[2]Institute of Technical Electronics, Technical University of Munich, Germany

Abstract

This work is an analytical description of a phenomenon known as electron emission from ferroelectrics. The production of free electrons from the surface of ferroelectrics with a metal lattice structure will be explained. An analytical field calculation shows that with a given structure the apparent surface charges of the ferroelectrics produce an electric field, which causes an electron emission from the metal lattice because of the tunnel effect. The emission process is described on the basis of the Fowler-Nordheim formula. After the polarization change of the ferroelectrics, free electrons are produced as a result of the Coulomb interaction. In theory this work analyzes the question of producing high density electron currents by means of ferroelectric materials. The calculated values are compared to empirically found data.

1 INTRODUCTION

First it should be stated that the experimental investigation of ferroelectrics in terms of electron emission is not new. After a fast pole-changing (≈ a few nano seconds) of the spontaneous polarisation P_S (Fig. 1) an intensive electron beam could be measured in a period of time ≈50 ns. About the causes (production of many free electrons) the above mentioned authors offered approaches yet no thorough descriptions of the phenomenon.

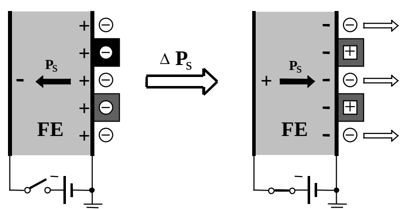

Figure: 1 Sketch of the pole change with subsequent emission of electrons from the surface

Next section it is assumed that the production of free electrons can be described as follows: It is shown that there is an equality of the measured emitted free charge carriers in the electron beam because of the Coulomb-repulsion (between the apparent surface charge density, the polarization of the ferroelectrics which was changed shortly beforehand, and the free charge carriers which tunnelled out of the metal for saturating the apparent surface charge density) and the apparent surface charges which in total of their charges correspond to the amount of charges tunneling out of the metal.

Hence, the interpretation of the cause of this phenomenon as described in this paper is contradictory to the approaches regarding the numerous free charge carriers in the electron beam to originate from an emission process out of the ferroelectrics. This phenomenon was observed by means of the test configuration below (Fig. 2).

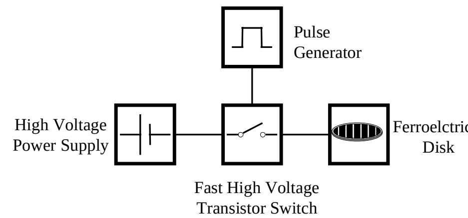

Figure: 2 Configuration used for electron production

The test configuration mainly consists of a pre-poled ferroelectric disk (Fig. 3), e.g. PLZT: 2/95/5, the backside completely coated with metal (gold) and the front side covered with a metal lattice layer (gold: line structure ≈200 µm).

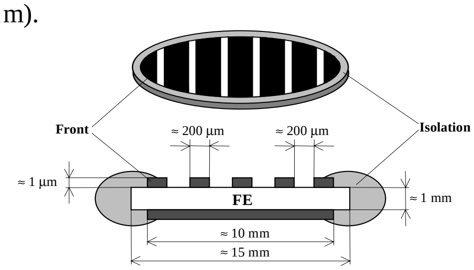

Figure: 3 Design of the FE-sample

Thus the disk acts as a capacitor. When applying a higher negative pulsed voltage (several kV) to the backside the shortly intensive (≈10 to 30 µC) electron beam (Fig. 5) was registred with a Faraday cup.

Considering a small latice hole to be a cylindrical bore hole (Fig. 3) in the metal of one of the capacitor plates (front), the electric field strength within the bore hole can be calculated for the time being for an uncompensated apparent surface charge density of the ferroelectric which in that place is uncovered and pre-poled.

On the basis of field emission, the density of the tunnel current coming out of the metal can be calculated using the Fowler-Nordheim formula. The differential equation for the compensation charges tunneling out (corresponds to the free charge carriers of the later on - after the change of polarization - emitted electron beam) can be integrated exactly and allows to state a relation between the apparent surface charge load, the period of half-life and the initial tunnel current density [1].

2 DETERMINATION OF THE POTENTIAL AND OF THE ELECTRIC FIELD STRENGTH

We consider two capacitor plates with the distance l between which there is a ferroelectric with the potential U_0. One of the capacitor plates has several cylindrical bore holes at regular distances which are relatively long as compared to the diameter of the bore hole; in other words: one single lattice segment is approximated by a cylindrical bore hole. We want to determine the electric field in the capacitor near a representative bore hole and in the bore hole itself (Fig. 4). The geometrical, electric influence of the other bore holes on the representatively selected one shall be neglected.

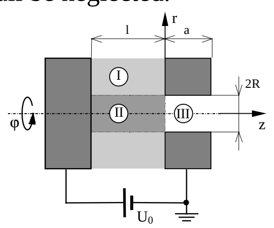

Figure: 4 Geometrical arrangement for the calculation of the electric field

After introducing cylindrical coordinates (z, r, φ) the potential function $v(r, z)$, which is to be determined and which is independent of φ both within the capacitor and in the bore hole itself in the general case, can be written as an infinite series over Bessel J_0 or Neumann functions N_0, respectively:

$$V(r,z) = (A + B\cdot z)\cdot(C + D\cdot\ln(r)) + \sum_n^{\infty}\left\{E_n \cdot J_0\left(\frac{J_{0_n}}{R}\cdot r\right) + F_n\cdot N_0\left(\frac{J_{0_n}}{R}\cdot r\right)\right\}\cdot \left\{G_n\cdot\exp\left(-\frac{J_{0_n}}{R}\cdot z\right) + H_n\cdot\exp\left(\frac{J_{0_n}}{R}\cdot z\right)\right\} \quad (1)$$

where J_{ON} are the (tabulated) zeros of the Bessel function, and R is the Radius of the bore hole.

The integration constants A, B, C, D, E_n, F_n, G_n, H_n have to be found through boundary and transition conditions. In order to describe the ferroelectric adequately in the parts I and II, the relation

$$\vec{D} = \varepsilon_0\cdot\vec{E} + \vec{P} = \varepsilon\cdot\vec{E} + \vec{P}_s \quad (2)$$

between the dielectric displacement D, the electric field strength E and the spontaneous polarization P_S is valid. Hence we assume that the absolute dielectric constant ε as well as the spontaneous polarization are constant.

After a few elementary transformations and taking transition conditions into account we come to the following formula for the potential in part III [2]:

$$V_{III}(r,z) = -2\cdot R\cdot\left(P_s + \frac{U_0}{l}\cdot\varepsilon\right)\cdot\sum_{n=1}^{\infty}\frac{J_0\left(\frac{J_{0_n}}{R}\cdot r\right)\cdot\exp\left(-\frac{J_{0_n}}{R}\cdot z\right)}{J_{0_n}^2\cdot J_0(J_{0_n})\cdot\left(\varepsilon_0 + \frac{\varepsilon}{\tanh(J_{0_n}\cdot l/R)}\right)} \quad (3)$$

hence using

$$E_{III_r}(r = R, z > 0) = -\left.\frac{\partial V_{III}(r,z)}{\partial r}\right|_{(r=R,z>0)} \quad (4)$$

for the r-component of the electric field strenght E_{IIIr} inside the cylindrical bore hole we receive

$$E_{III_r}(r = R, z > 0) = 2\cdot\left(P_s + \frac{U_0}{l}\cdot\varepsilon\right)\cdot\sum_{n=1}^{\infty}\frac{\exp\left(-\frac{J_{0_n}}{R}\cdot z\right)}{J_{0_n}\cdot\left(\varepsilon_0 + \frac{\varepsilon}{\tanh(J_{0_n}\cdot l/R)}\right)} \quad (5)$$

In the case of

$$P_S \approx 10^4\cdot\varepsilon_0\cdot\frac{U_0}{l} \approx \frac{30\mu C}{cm^2}$$

the electric field strength amounts to approximately $2\cdot 10^8$V/cm. Using formula (5) we can find the electric field strength on the inner metal edge which on the basis of tunnel effect enables the metal electrons to overcome the work function.

3 CURRENT DENSITY AS A RESULT OF THE TUNNEL EFFECT

In quantum mechanics, the calculation of the permeability factor D is well known, and for the movement of an electron with the energy W through a potential energy barrier $U=U(x)$ is given by

$$D \approx \exp\left(-\frac{2}{\hbar}\cdot\int_{x_1}^{x_2}\sqrt{2\cdot m_e\cdot(U(x) - W)}\,dx\right) \quad (6)$$

In our situation, the barrier $U=U(x)$ is determined by the Fermi energy W_F and the work function on the one hand, and by the applied electric field E on the other hand.

$$U(x) = -E_{III_r}\cdot x\cdot e_0 + W_0 \quad (7)$$

Inserting $U(x)$ into the fundamental formula (6) of quantum mechanics for the tunnel effect, and after simple integration we finally arrive at

$$D = \exp\left(-\frac{2}{3\cdot\hbar\cdot m_e\cdot E_{III_r}}\cdot\sqrt{(2\cdot m_e\cdot(W_0 - W))^3}\right) \quad (8)$$

The electric field strength found in the above paragraph and for the work function W_0 the permeability factor e.g. for copper amounts to $4{,}2\cdot 10^{-8}$. Here the potential barrier is approximately as wide as four times the Bohr radius. When applying an electric field strength to a metal some electrons tunnel according to the permeability formula (6) from the metal into the vacuum so as to compensate the positive unfree apparent charge of the high spontaneous polarization in terms of absolute value. In order to estimate how fast the compensation effect goes it is necessary for the time being to determine the current density J_T of the electrons tunneling out. It is known that the current density results from the Fermi distribution of the electrons in metal and from the permeability formula (6), giving the Fowler-Nordheim formula.

$$J_T = \frac{e^3\cdot E_{III_r}}{h\cdot 8\pi\cdot(W_0 - W_F)}\cdot\exp\left(-\frac{2\cdot\sqrt{(2\cdot m_e\cdot(W_0 - W_F))^3}}{3\cdot\hbar\cdot m_e\cdot e\cdot E_{III_r}}\right) \quad (9)$$

Writing the electric field strength E_{IIIr} in V/m, the work function W_A in eV and the tunnel current density J in A/m^2 the Fowler-Nordheim formula in dimensionless quantities to be measured reads:

$$J_T = 1{,}54\cdot 10^{-6}\cdot\frac{E_{III_r}^2}{W_A}\cdot\exp\left(-6{,}826\cdot 10^9\cdot\frac{\sqrt{W_A^3}}{E_{III_r}}\right)\ \text{in}\ \left[\frac{A}{m^2}\right] \quad (10)$$

Again inserting in (10) the electric field strength of our example and the work function W_A of copper for the tunnel current density amounts to approximately 1200 A/cm^2 and is the higher the shorter the period is. Moreover, we note that a slight increase in the electric field strength immediately results in a considerably higher tunnel current density and hence, as will be explained in the following paragraph, there is just a faster compensation of the apperent surface charges by the electrons tunneling out of the metal.

4 SATURATION OF THE FERROELECTRIC SURFACE IN TERMS OF TIME

The relations (5) and (9) allow us to write a differential equation for the still uncompensated apparent surface current density $\eta_S(t)$

$$\eta_s(t) = \eta_s - \frac{Q(t)}{\pi \cdot R^2} \tag{11}$$

where $P_S = \eta_S(t=0) = \eta_S$ and $Q(t)$ is the charge which tunneled out of the metal by the time t:

$$J_T(t) \cdot a \cdot 2\pi \cdot R = \frac{dQ}{dt} = a \cdot 2\pi \cdot R \cdot \frac{6{,}2 \cdot 10^{-6}}{11{,}1} \cdot \sqrt{\frac{7{,}1}{4}} \cdot \left(\varepsilon \cdot \frac{U_0}{l} + \eta_s(t) \right)^2 \cdot$$

$$\sigma^2 \cdot \exp\left(- \frac{6{,}8 \cdot 10^9 \cdot \sqrt{4^3}}{\left(\varepsilon_0 \cdot \frac{U_0}{l} + \eta_s - \frac{Q(t)}{\pi \cdot R^2} \right) \cdot \sigma} \right) \tag{12}$$

Here a means the depth of the bore hole, and σ is a shortcut for the following:

$$\sigma = -2 \cdot \sum_{n=1}^{\infty} \frac{\exp\left(- \frac{J_{0_n}}{R} \cdot z \right)}{J_{0_n} \cdot \left(\varepsilon_0 + \frac{\varepsilon}{\tanh(J_{0_n} \cdot l / R)} \right)} \tag{13}$$

After introducing further suitable shortcuts

$$\Psi = \left(\varepsilon \cdot \frac{U_0}{l} + \eta_s \right) \cdot \pi \cdot R^2 \,, \quad \Omega = \frac{M}{\pi^2 \cdot R^4} \cdot \frac{6{,}2 \cdot 10^{-6}}{11{,}1} \cdot \sqrt{\frac{7{,}1}{4}} \cdot \sigma$$

$$\Phi = \frac{6{,}8 \cdot 10^9 \cdot \sqrt{4^3} \cdot \pi \cdot R^2}{\sigma} \tag{14}$$

our differential equation can be transformed as follows

$$\frac{dQ}{dt} = \Omega \cdot (\Psi - Q)^2 \cdot \exp\left(- \frac{\Phi}{\Psi - Q} \right) \tag{15}$$

It can be solved by separation of the variables, and using the inititial condition $Q(t=0)=0$ (by the time t=0 there has been no tunnel charge emission) we get

$$Q(t) = \Psi - \frac{\Psi}{\ln\left(\Phi \cdot \Omega \cdot t + \exp\left(\frac{\Phi}{\Psi} \right) \right)} \tag{16}$$

We note that $Q(t = \infty) = \Psi$. As the standard for the time behaviour of the compensation we use half-life τ:

$$\tau = \frac{1}{\Phi \cdot \Omega} \cdot \exp\left(\frac{\Phi}{\Psi} \right) \cdot \left(\exp\left(\frac{\Phi}{\Psi} \right) - 1 \right) \tag{17}$$

Inserting the values of our example in (17) results in $\tau = 4\ 10^{-4} ns$, i.d. in a very short period of time a considerable part of the apparent surface charge density will be saturated by the electrons tunneling out of the metal. Finally, since we arrive at

$$\exp\left(\frac{\Phi}{\Psi} \right) \approx 15 >> 1 \tag{18}$$

in our example an approximated formula for τ is:

$$\tau = \frac{1}{\Phi \cdot \Omega} \cdot \exp\left(\frac{\Phi}{\Psi} \cdot 2 \right) \tag{19}$$

Moreover, (12) in combination with (16) at $t=0$ provides the tunnel current density. Since Φ and Ω are independent of the apparent surface charge density η_S we get a relation which combines η_S with τ and $J_T(t=0)$:

$$\eta_s \cdot \pi \cdot R^2 = \sqrt{\sqrt{\tau} \cdot J_T(t=0) \cdot M \cdot \sqrt{\frac{\Phi}{\Omega}}} \tag{20}$$

Formula (20) shows the relations between relevant quantities in the compensation process as a result of the tunnel effect. After fast pole change ($P_S \rightarrow -P_S$) the compensation charges are suddenly confronted with apparent surface charge densities with the same sign and are hence repelled. A corresponding pulse of current $I_M(t)$ if integrated over time is then exactly

$$\eta_S \cdot \pi \cdot R^2 = \int_{t=0}^{\infty} I_M(t)\, dt = \bar{I}_M \cdot t_M \tag{21}$$

the previous compensation charge. Thus, we showed in this paper that compensation charges can appear mainly as a result of the tunnel effect from the metal of the capacitor charge. We get

$$\bar{I}_M \approx \frac{1{,}8}{5} A$$

which corresponds with the data measured [3].

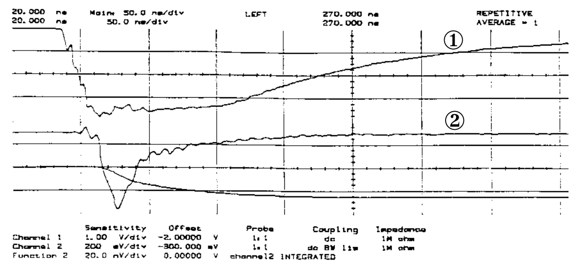

Figure: 5 The sample response ② to a negative pulse applied to the backside ①

5 CONCLUSION

The results of this paper allow to conclude that the problem of the place where the compensation charges for the saturation of high apparent surface charge densities in ferroelectric materials come from has a relative simple solution. The physical explanation is that the apparent surface charges of the ferroelectric create very strong electric fields within the lattice holes, with the lattice having a potential of $V=0$. These fields cause the emission of electrons from the metal lattice (quantum mechanic tunnel effect). These electrons create the compensation charges, so that after the pole change of the ferroelectric ($V=-U_0$) they can be registered [4] as free charge carriers in the electron beam (as a result of the Coulomb force between the apparent charges and the compensation electrons).

REFERENCES

[1] H. Heydari: "Analytical description of a phenomenon known as electron emission from ferroelectrics", TET-Note 91/006, Technical University of Berlin, 1991.

[2] T. Tille: "Pollutant free emission of exhaust fumes based on a pulsed ferroelectric high current electron source", Diploma thesis, Technical University of Berlin, April 1995.

[3] H. Gundel, H. Heydari, D. Suchland, K. Schmidt, H. Henke: "Profile Measurements on a Pulsed Ferroelectric Electron Beam", EPAC'92, pp. 1023-1025, Berlin, March 1992.

[4] D. Suchland, F. Heinrich, H. Heydari: "Temperature dependence of electron emission from PLZT by laser induced switching", TET-Note 91/007, Technical University of Berlin, 1991.