Erciyes Üniversitesi Fen Bilimleri Enstitüsü Dergisi **21** (1-2), 24-2 9, 2005

CAPACITANCE STUDY OF FERROELECTRIC P-N JUNCTION

Mehmet S. BOZGEYIK

Department of Physics, Kahramanmaras Sutcuimam University, 46100, Kahramanmaras-TURKEY

ABSTRACT

Capacitance study of ferroelectric *pn* junction having uneven interface was theoretically carried out in case of two dimensional (2D) spontaneous polarization by means of Phenomenological Theory of Ferroelectricity and electrostatics. From the Gauss Law we calculated capacitance via calculation of polarization and electric potential in the depletion region of junction in ferroelectric and paralectric phases. We evaluate dimensionless junction capacitance upon change of temperature and voltage by designation of dimensionless parameters. This model especially deals with semiconductor ferroelectrics.

Keywords: Ferroelectric, *pn* junction, Junction capacitance, Spontaneous Polarization, Semiconductor ferroelectric, Phenomenological theory of ferroelectricity.

FERROELEKTRİK P-N EKLEMIN SIĞA ÇALIŞMASI

ÖZET

Düzgün olmayan arayüzeyli ferroelektrik *pn* eklem sığa çalışması iki boyutlu (2B) spontan (kendiliğinden) kutuplanma durumunda Ferroelektrikliğin Fenomenolojik Teorisi ve elektrostatik kullanılarak teorik olarak yapıldı. Eklemin sızma bölgesindeki sığasını Gauss Yasasıyla toplam polarizasyon ve elektrik potansiyeli hesabı üzerinden ferroelektrik ve paraelektrik fazda hesapladık. Tanımlanan birimsiz parametrelerle sıcaklık ve gerilim değişimi ile birimsiz eklem kapasitansını değerlendirdik. Bu model özellikle yarıiletken ferroelektrikleri ele almıştır.

Anahtar Kelimeler: Ferroelektrik, *pn* eklem, Eklem sığası, Kendiliğinden kutuplanma (Spontan polarizasyon), Yarıiletken ferroelektrik, Ferroelektrikliğin fenomenolojik teorisi.

E-posta: msbozgey@yahoo.com

1. INTRODUCTİON

Semiconductor ferroelectrics are of great importance in ferroelectricity from the point of view of the influence of electron subsystems to the phase transition and vice versa. Moreover, analysis of two dimensional electron systems is especially important from the viewpoint of that such systems are used in microlectronic and optoelectronic devices. Furthermore, relationship among spontaneous polarization and electron subsytems in electronic structures for instance, *p-n* junction, which is the main component of many microelectronic devices, gives rise interesting behavior upon variation of temperature and other external effects. A *p-n* or Schottky diode consits of a junction capacitance, a junction conductance, and a series resistance [1]. The depletion layer capacitance accounts for most of the junction capacitance when the junction is reverse biased [2]. Unlike the case of a parallel plate capacitor the stored charge in the depletion region does not depend linearly on the voltage [3]. Junction capacitance is one of the important measurables of such systems. Petrosyan, S. et al. theoretically showed that junction capacitance varies logarithmically with the applied voltage for such a 2D *p-n* junction[4]. Although many proposed new geometries require the growth of high quality films, kinetic effects may induce random roughness formation depending on the growth conditions [5]. Consequently, deviations of surface and interface from flatness as well as the presence of defects (e.g. dislocations, impurities, etc.) may alter the operation of microelectronic devices [3, 6]. Therefore, influence of interface morphology on the electrical conductivity of semiconducting films was shown in many studies. For instance, considerable research is devoted to understand the electrical properties of devices affected by these imperfections, which might otherwise prevent device applications such as storage capacitors for dynamic and static random access memories [5]. For a Non-Volatile Ferroelectric Random Access Memory (NV-FeRAM) ferroelectric serves not just as capacitor, but as the memory element itself [7]. In fact, capacitance calculations and measurements are of great importance in realization and application of this device. Due to metalic electrodes ferroelectric thin film capacitors can be viewed as three capacitors in series, the two Schottky capacitors formed at the interfaces and the bulk capacitors. Mathematically, voltage dependence of interface capacitance were discussed for such a system [8]. Moreover, temperature dependence of interface capacitance properties were experimentally studied by considering series capacitor model [9] for ferroelectric thin film capacitors [10, 11]. In present study, junction capacitance of ferroelectric *p*-n junction having corrugated interface is theoretically calculated by means of phenomenological theory of ferroelectricity and electrostatics.

2. THEORETİCAL RESULTS AND DİSCUSSİON

Since almost all of the physical properties of a *p-n* junction are related to the space charge region [12], one needs to solve Maxwell or Poisson equations in order to derive the distribution of electric field and potential, and for calculations of other physical quantities in depletion region. We consider a ferroelectric *p-n* junction which has not smooth interface. For mathematical simplicity we model this roughness as sinusoidal 2D corrugation aligned in *y*-axis according to the geometry of *p-n* junction as sketched in Figure 1. In our spacial case polar axis is directed on *x*-y plain. So, with regard to geometry of problem we deals with 2D spontaneous polarization. Two dimensional corrugation is described by a function $x(y) = x_0 Cosky$.

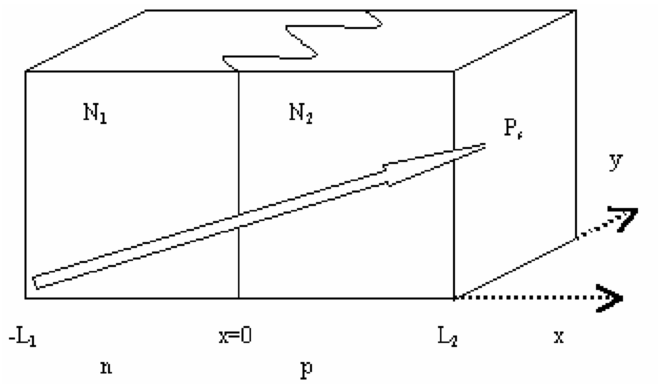

Figure 1. Sketch of space charge region of ferroelectric *p-n* junction having corrugated interface with 2D spontaneous polarization alignment.

Suppose that electric field is small enough i.e. ($\varepsilon_0 \boldsymbol{E} << \boldsymbol{P}$). Consequently, one can write $\boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P} \cong \boldsymbol{P}$. So, the Gauss law states

$$\nabla.\boldsymbol{D} = \nabla.\boldsymbol{P} = \rho \tag{1}$$

Here, $\rho = q(N_1 - N_2 + Q)$ where $\boldsymbol{q}$ is the magnitude of electronic charge, N_1 and N_2 are ionized donor and acceptor concentrations, respectively, and $Q = (p - n)$ stands for the difference of hole and electron concentrations. By solving (1) in one dimension (in *x*-axis) one finds total polarization as

$$P(x) = \pm qN_{1,2}(x \pm L_{1,2}) + P_{sx} \tag{2}$$

where $L_{1,2}$ is the space charge boundaries in respected regions and P_{sx} is *x*-component of spontaneous polarization. As seen in (2), total polarization is combination of induced polarization and spontaneous one. Suppose that the amplitude of spatial corrugation $\boldsymbol{x_0}$ is small compared to the length of space charge region. Therefore, one can expand total polarization (2) in Taylor series at *x*=0 around x_0. Hence, for the first order approximation $P(x_0) + (x - x_0)\frac{dP}{dx}\Big|_{x_0}$ one ends up with $\pm qN_{1,2}(x \pm L_{1,2}) + P_{sx}$. Consequently, we ignore effect of roughness in *x*-axis calculations. On the other hand, we should not disregard influence of corrugation on polarization, potential energy, etc. through interface in *y*-axis .

Besides electrostatic calculations we have performed Phenomenological Theory of Ferroelectricity for this study. We consider a semiconductor ferroelectric, which has second order phase transition, constitute *p-n* junction. Therefore, one expands elastic Gibbs free energy in even power series of spontaneous polarization

$$G_1 = G_{10} + \frac{1}{2}\alpha P_{sx}^{\;2} + \frac{1}{4}\beta P_{sx}^{\;4} \tag{3}$$

where G_{10} is the free energy in paralectric phase $\alpha = \frac{2\pi}{C_0}(T - T_c)$, T_c phase transition temperature (the Curie point) , C_0 Curie-Weiss constant and β is a constant. Electric field is derived as

$$E = (\frac{dG_1}{dP_{sx}}) = \alpha P_{sx} + \beta P_{sx}^{\;3} + ... \tag{4}$$

Consider that reverse bias is applied to the system. Assume that the boundary conditions are follows $V(-L_1) = 0$ and $V(L_2) = -V$, and $P(-L_1) = P(L_2) = P_{sx}$. From (1) total polarization of each side of space charge region is found as

$$P(x) = \begin{cases} qN_1(x + L_1) + P_{sx}, & x < 0 \\ -qN_2(x - L_2) + P_{sx}, & x > 0 \end{cases} \tag{5}$$

Note that total polarization is described as combination of induced and spontaneous polarization as $P(x) = P_{ind}(x) + P_{sx}$ and $P_{sx} >> P_{ind}(x)$. By using (4) one derives potential energy in terms of spontaneous polarization and a dimensionless parameter designated as $p = \frac{\left\| P_{ind}(x) \right| - \left| P_{sx} \right\|}{P_{sx}}$.

$$U(x) = -qV(x) = \begin{cases} \frac{\beta P_{sx}^4}{4N_1}(p^2-1)^2, & x \le 0, \\ qV - \frac{\beta P_{sx}^4}{4N_2}(p^2-1)^2, & x \ge 0, \end{cases} \tag{6}$$

Equating the potential energy at interface yields

$$(p_0^2 - 1)^2 = \frac{4qNV}{\beta P_{sx}^4} = A^2 \tag{7}$$

which is a nonlinearty parameter of the system, where $N^{-1} = N_1^{-1} + N_2^{-1}$. From the boundary condition of spontaneous polarization and (5) only valid solutions of four roots of (7) is found as $p_0 = \sqrt{1+A}$. Since polarization is continues at interface by using (5) one obtains

$$\frac{qN_1L_1}{P_{sx}} = \frac{qN_2L_2}{P_{sx}} = p_0 - 1 \tag{8}$$

Let us designate two more dimensionless parameter related to potential and temperature as follows $v = \frac{V}{\overline{V}}$, where $\overline{V} = (\frac{\pi T_c}{C_0})^2 \frac{1}{q\beta N}$ [13, 14] and $t = \frac{T}{T_c}$. Hence, one rewrites A^2 in a following form

$$A^2 = \frac{4qNV}{\beta P_{sx}^4} = \frac{v}{(1-t)^2} \tag{9}$$

Now, we can express the *p-n* junction capacitance related to the derivation of space charge length with respect to the applied voltage as

$$C_{pn} = \frac{dQ}{dV} = qN_2(\frac{dL_2}{dV}) \tag{10}$$

Assume that a unit capacity as $\overline{C} = (\frac{C_0}{2\pi T_c})^{3/2} qN\beta^{1/2}$ [13,14]. From (8) one writes $qN_2L_2 = P_{sx}(p_0 - 1)$. By using $p_0 = \sqrt{1+A}$ it is obtained $qN_2L_2 = P_{sx}((1+A)^{1/2} - 1)$. Now, we are able to incorporate dimensionless parameters in remaining equations

$$qN_2L_2 = P_{sx}((1-t)^{-1/2}(1-t+v^{1/2})^{1/2} - 1) \tag{11}$$

If we differentiate above equation and derive the differential form of potential by using (9) we obtain

$$C_{pn} = \frac{qN}{\beta P_{sx}^3}(v(1-t+v^{1/2}))^{-1/2} \tag{12}$$

and dimensionless parameter related to capacitance is obtained by using unit capacity

$$c_F(t,v) = \frac{C_{pn}}{\overline{C}} = \left\{ v(1 - t + v^{1/2})\right]^{-1/2}, t \leq 1. \tag{13}$$

Variation of c_F with respect to temperature and potential is plotted in Figure 2.

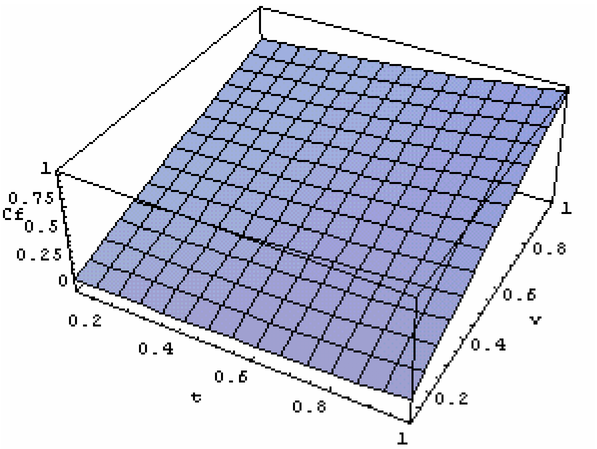

Figure 2. Plot of dimensionless capacitance with respect to temperature and potential in ferroelectric phase.

Analogously, in paraelectric phase with the boundary condition $P(-L_1) = P(L_2) = 0$ one obtains $p_0 = [(1 + A^2)^{1/2} - 1]^{1/2}$, where $p_0 = \frac{qN_2L_2}{p_p}$ and $A^2 = \frac{4qNV}{\beta P_p^4}$. Here, $p_p = (\frac{\alpha}{\beta})^{1/2}$ is such a polarization rather than spontaneous one. Therefore, capacitance of *p-n* junction is derived as

$$C_{pn} = \frac{qN}{\beta P_{sx}^3}(((t-1)^2 + v)^{3/2} - (t-1)((t-1)^2 + v))^{-1/2} \tag{14}$$

And finally we end up with

$$c_P(t,v) = \frac{C_{pn}}{\overline{C}} = \left\{ [(t-1)^2 + v]^{3/2} - (t-1)[(t-1)^2 + v]\right\}^{-1/2}, t \geq 1. \tag{15}$$

Evaluation of c_P with variation of temperature and voltage is depicted in Figure 3.

On the other hand, together with *y*-component of spontaneous polarization roughness, which is modeled as periodic corrugation along the interface, may cause accumulation of charges at interface. Hence, charge distributions possibly changes at rough interface due to such charge accumulation. Although this may alter the junction capacitance of system, the effect of morphology on junction capacitance needs accurate studies for further discussion. Furthermore, such imperfection of morphology of interface possibly yields degradation of current, and influences related transport mechanism of device applications. Once again we will investigate such speculations with further accurate analytical studies soon.

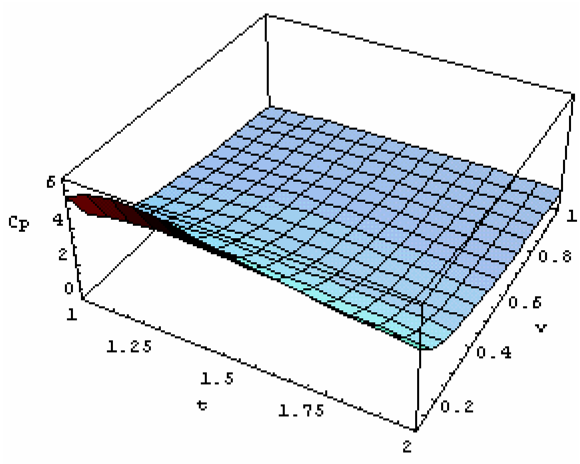

Figure 3. Depict of dimensionless capacitance with variation of temperature and voltage in paraelectric phase.

3. CONCLUSİON

To summarise, capacitance of ferroelectric *p*-n junction having corrugated interface with 2D spontaneous polarization were analytically investigated by means of Phenomenological Theory of Ferroelectricity and electrostatics for both ferroelectric and paraelectric phases in current study. By definitions of dimensionless parameters we were allowed to easily evaluate capacitance and other related physical measurables upon change of temperature and voltage. It was observed that in ferroelectric phase capacitance increases with increasing temperature and voltage. On the contrary, in paraelectric phase, firstly, it increases and has a maximum value, and then decreases with increasing temperature. Also, it decreases with increasing external voltage. Under special circumstance we ignore the possible effect of imperfection to capacitance. We carried out calculations disregarding influence of roughness in the perpendicular direction of component of spontaneous polarization with respect to the plane of junction interface. Through the parallel direction of interface plane respected component of spontaneous polarization deflects charges and gives rise such a accumulation. Also, we speculate that together with the effect of morphology this may change the capacitance and cause some side effects in transport mechanism of such ferroelectric *p-n* junction devices.

REFERENCES

1. Schroder, K. Dicter, Semiconductor Material and Device Characterization, John Wiley&Sons, Inc. New York, 1990.
2. Kasap, S. O., Priciples of Electronic Materials and Devices, Mc Graw Hill, New York, 2002.
3. Sze, S. M., Semiconductor Devices: Physics and Technology, Jhon Wiley & Sons, Inc. New York, 2002.
4. Petrosyan, S. et al., Appl. Phys. Lett. **84**, 3313-3315, 2004.
5. Palasantzas, G. and De Hosson, J. Th. M., , Solid State Commun. **118**, 203, 2001.
6. McKinley, K. A., Sandler, N. P. Thin Solid Films **290**, 440, 1996.
7. Scott, J. F., Ferroelectric Memories, Springer-Verlag Berlin 2000.
8. Meng, X. J. Et al., Appl. Phys. Lett. **78**, 2548-2550, 2001.
9. Sinnamon, L. J., et al. Appl. Phys. Lett. **78**, 1724-1726, 2001.
10. Mcaneney, J., et al. Integrated Ferroelectrics **60**, 79-86, 2004.
11. Lookman, A., et al. Integrated Ferroelectrics **61**, 51-58, 2004.
12. Grove, A. S, Physics and Technology of Semiconductor Devices, John Wiley and Sons, Inc., London, 1967.
13. Sandomirskii, V.B. et al., Sov. Phys. Semicond. **16**(3), 279, 1982.
14. Sandomirskii, V.B. et al., Ferroelectrics **45**, 107, 1982.