A New Physical Model for the Relaxation in Ferroelectrics

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Abstract

The loss of polarization in ferroelectric capacitors due to the relaxation of the dipoles was measured with a simple procedure in the range between 1µs and 10s. Physical considerations lead to a quantitative model for the relaxation process. This new model is based on the Preisach-Everett approach. The model was implemented in a circuit simulator. Simulations and measurements show good agreement. The simulation of a FRAM-cell shows that the bit line signal declines by 10% within the first 10s.

1. Introduction

The most commonly used description for polarization in ferroelectric materials is based on the Preisach-Everett model for ferromagnetics, which is described e.g. in [1]. Its implementation into circuit simulators was performed by Bo Jiang [2].

So far, however, time related phenomenons have not been included into this model. Even with no external voltage applied to the ferroelectric some loss of polarization will take place, due to the thermodynamic instability of the dipoles. This relaxation was observed e.g. by Shimada [3] and Moazzami [4].

2. Measurement

For our measurements of polarization loss testing capacitors of strontium-bismuth-tantalate (SBT) with two different sizes (100µm² and 40µm²) were used. The polarization on the ferroelectric capacitor was established with a Sawyer-Tower-Circuit (Fig.1). An initial pulse with 50µs period ensured that the whole ferroelectric was polarized in down direction. After a waiting time that ranged between 2µs and 10s, a second pulse of the same period was applied to measure the relaxed polarization. As can be seen in Fig. 2, the difference of the voltage DV_O is only dependant on the polarization of the ferroelectric capacitor.

Figure 3 shows the results of our measurements. The linear contribution of the dipoles which is not affected by relaxation was subtracted. The measured polarization is referred to the remanent polarization.

Both of the tested capacitors show the same loss of polarization over time. The

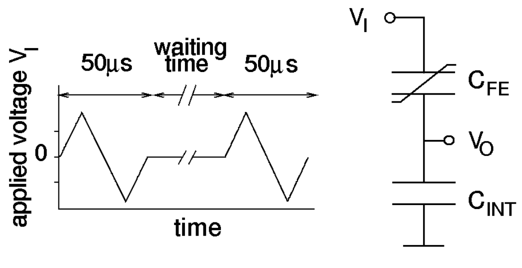

Fig.1:The 50µs pulse is applied at V_I, the charge is measured at V_O

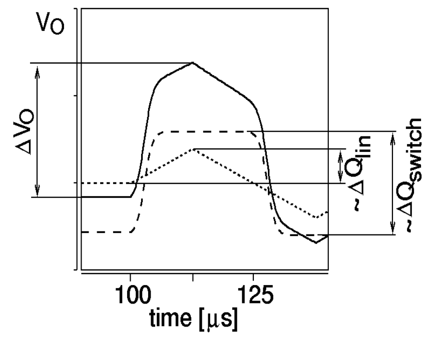

Fig.2: The charge on C_{FE} (Q_{switch}: switching dipoles, Q_{lin}: linear dielectric term) is measured by ΔV_O

decay exhibits a logarithmic time dependence which suggests that the time constants for the relaxation have a distribution over some orders of magnitude. This is in agreement with the observations in [3].

3. The model

3.1. The original Preisach model

The basic idea of the Preisach model is, that the ferroelectric material consists of a set of individual dipoles that contribute to the total polarization. Each of these dipoles has two individual coercive voltages, v_{c+} and v_{c-}, that are required to make it switch into the opposite direction. Thus each dipole has a rectangular hysteresis loop (Fig. 4). Based on the assumption that the dipoles are non-interacting the hysteresis loop of the macroscopic system is seen as a superposition of these hysteresis units.

v_{c+} and v_{c-} of the hysteresis units in the macroscopic system are statistically distributed.

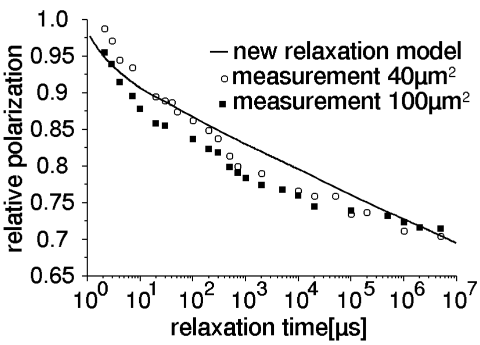

Fig.3: Relaxation of polarization

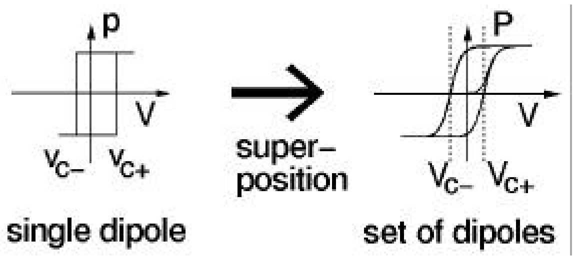

Fig.4: Hysteresis loop

The concept is best explained by an example (Fig. 5). Initially all dipoles are in down polarization . Then the external voltage rises to the value V_2 and the dipoles with $v_{c+} < V_2$ will switch to up position, whereas the dipoles with $v_{c+} > V_2$ remain in down position. Now the voltage is decreased to a value V_3. As before dipoles with $v_{c-} > V_3$ will switch back to down position, whereas those with $v_{c-} < V_3$ maintain their up position. Now, however, the dipoles that remained in down position after the first step do not participate in the switching process of the second step as they have conserved their down position.

So the distribution of the dipoles to their up and down states is dependant on the voltage turning points. The total polarization P of the ferroelectric results in:

p is the polarization of a single dipole,

$$P(V,V_1,V_2,...)= \iint_{v_{C+}v_{C-}} r(v_{C+}v_{C-})D(V,V_1,V_2,...)\cdot p\,dv_{C+}dv_{C-} \qquad (1)$$

r (v_{c+},v_{c-}) the density function of the dipoles with respect to their individual coercive voltages and D a direction operator (± 1) depending on the actual voltage and the turning points it has passed.

The tanh-function is a useful approximation for the integral in (1) when r is taken as a Gauss distribution:

$$P(V) = F \cdot P_{Sat} \cdot \tanh[a(V \mp V_{C\pm})] \qquad (2)$$

P_{Sat} is the saturation polarization and $V_{C\pm}$ is the macroscopic coercive voltage, i.e. the mean value of the individual coercive voltages. The behaviour of the non-saturation loops are taken into account by a factor, so

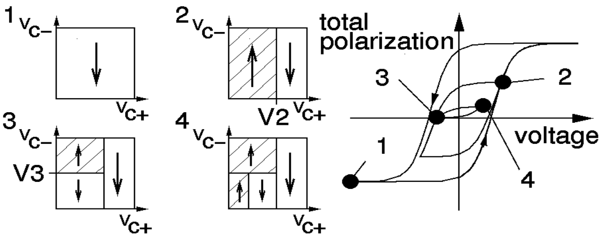

Fig.5: The dipoles are classified by *(v_{c+}, v_{c-})*. The history of external voltage determines the state of each dipole

that $F \times P_{Sat}$ represents that proportion of dipoles that take part in the switching process of the non-saturation loop. This is the well-known model described by Bo Jiang [2].

3.2. Modelling relaxation

So far the only force that provokes the switching of the dipoles was the external electric field. But there are other forms to provide the activation energy for switching. One of the essential ones is thermal activation. This means that the ferroelectric material strives for a thermal equilibrium with a certain proportion of the dipoles switched to the other state. So the relaxation of polarization without external field takes place.

First a subset n_i of dipoles with the probability w_{+i} for switching to the up-state and w_{-i} for switching to the down state is examined. The evolution of the total polarization is calculated from

$$\frac{dP}{dt} = w_{+i} \cdot n_{\downarrow i} \cdot p - w_{-i} \cdot n_{\uparrow i} \cdot p \qquad (3)$$

where p is the polarization of a single dipole, n_{-i} and n_{-i} the amounts of dipoles in the up- and down-state respectively. After solving the differential equation and assuming that the total amount of dipoles n_i is initially in the down-state, the following time-dependant polarization results:

$$P(t) = p \cdot (n_{\uparrow i}(t) - n_{\downarrow i}(t)) = n_i p \cdot \frac{w_{+i} - w_{-i}}{w_{+i} + w_{-i}} -$$
$$n_i p \cdot \left(\frac{2 w_{+i}}{w_{+i} + w_{-i}} \cdot \exp\left\{ - \frac{w_{+i} + w_{-i}}{2} \cdot t \right\} \right) \qquad (4)$$

The factor in the exponent represents the decay time t_i for this subset of dipoles and the subtrahend is the final polarization at t=¥. Now w_+ and w_- are calculated by assuming a Maxwell distribution *f(E)* for the inner energies of the dipoles. For simplification only the exponential tail of the Maxwell distribution is used:

$$w_{\pm i} = \frac{\int_{E_{A\pm}}^{\infty} f(E) dE}{\int_0^{\infty} f(E) dE} \approx B \cdot \exp\{- b \cdot E_{A\pm}\} \qquad (5)$$

$E_{A\pm}$ is the activation energy in the subset that has to be exceeded when switching occurs. $E_{A\pm}$ has a certain relation to $v_{c\pm}$. We found that a quadratic dependence gives good results:

$$w_{\pm i} \approx A \cdot \exp\{- a \cdot v_{C\pm}^2\} \qquad (6)$$

A and a are fitting parameters. The wide variety of decay times (Fig. 3) becomes now apparent: the decay time in (4) depends on the switching probability $w_\pm$ with its exponential dependence on the activation energy (5,6).

Now the total set N of dipoles is examined: Figure 6 shows the Preisach picture of such a relaxation process. The total set of dipoles N is subdivided into subsets n_i with characteristic $w_{\pm i}$'s. If $a \geq 20$ the following simplifications are valid:

$v_{C\pm}$	$w_{\pm i}$	decay time τ_i	final state $P(t=\infty)$
$v_{c-} < v_{c+}$	$w_{-i} >> w_{+i}$	$\tau_i = 2/w_{-i}$	$-n_i \cdot p$
$v_{c-} \approx v_{c+}$	$w_{-i} \approx w_{+i}$	$\tau_i = 1/w_{\pm i}$	0
$v_{c-} > v_{c+}$	$w_{-i} << w_{+i}$	$\tau_i = 2/w_{+i}$	$+n_i \cdot p$

In our example (Fig. 6) the dipoles are initially in down-state. The front of dipoles relaxing to the up-state moves from high w_+ to low w_+ and is governed by the respective t. The exponential dependence of t on v_{c+} has to be born in mind to see that

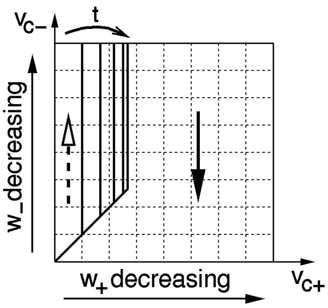

Fig.6: Initially in down-state, the dipoles with high w_+ switch to up state.

the relaxation process takes place over orders of magnitude in time.

As *t* from thermal activation increases rapidly, other effects are dominant for the depolarization in the longer time range.

4. Implementation to Simulator

The Preisach model without relaxation is implemented in a circuit simulator by storing the voltage turning points (Fig. 5) [2]. By these turning points the amounts of dipoles in the up- and down-states are unambiguously defined.

Relaxation also produces such a well defined, now time-dependent, distribution. This distribution is generated in the simulation by "artificial" voltage turning points. For every time step, the location of the extremes is calculated with (4) and the total polarization is adjusted to this new value.

The good agreement between simulation and measurements (Fig. 3) was be achieved by using five artificial turning points only.

5. Application: FeRAM

With our new relaxation model predictions for FeRAM-cells in memory arrays can be performed. Fig 7 shows simulations where a 0.35µm²-FeRAM cell is evaluated at a bit line with a 100fF parasitic capacitor. The decline of the bit line signal results in about 10% within 10s. This has to be

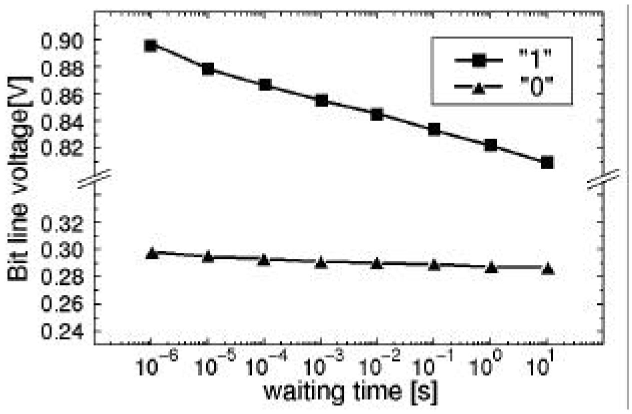

Fig. 7: Simulation: A 0.35µm² FRAM-cell is read after different waiting times.

taken into consideration for accurate FeRAM modelling.

6. Conclusion

The relaxation of polarization in ferroelectric capacitors has been measured. The logarithmic decay of polarization was modelled by a development of the standard Preisach model. It was refined by inserting the thermodynamic activation energy resulting in a time-dependent model. This new model was implemented in the circuit simulator that showed good agreement with measurement. The modelling of relaxation is imperative for accurate prediction of FeRAM-performance.

7. References

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