Transient Simulation of Ferroelectric Hysteresis

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ABSTRACT

We present a model that allows the analysis of the behavior of ferroelectric materials in a wide range of frequencies. A common approach to the transient properties of dielectrics based on differential equations was extended by an additional term representing the nonlinearity of the material. Our model was designed with respect to a stable discretization. Based on a transient formulation, our model allows the analysis of the device in the time regime. This includes the simulation of relaxation, thus enabling an exact analysis of the read and write cycles of ferroelectric nonvolatile memory cells. As an example the parameters for a specific device were extracted using measured data and an excellent correspondence was achieved.

Keywords: hysteresis, frequency dependence, ferroelectric materials, nonvolatile memory

1 Introduction

During recents years ferroelectric materials became more and more attractive for usage in nonvolatile memory cells. Increasing clock frequencies lead into a regime where the frequency dependence of basic material parameters like coercive field and remanent polarization can no longer be neglected. At high frequencies, the hysteresis widens and the coercive field increases, which is of fundamental interest for the extraction of parameters for write and read cycles like applied voltage or pulse length.

2 Modeling

For precise simulation we have developed an appropriate model which allows the analysis of the transient behavior. Simulation in the frequency regime would be numerically less complex, but leads to reduced capabilities in comparison with the time regime. Especially in the context of arbitrarily shaped signals and relaxation effects the rigorous approach of our simulator MINIMOS-NT[1] is mandatory.
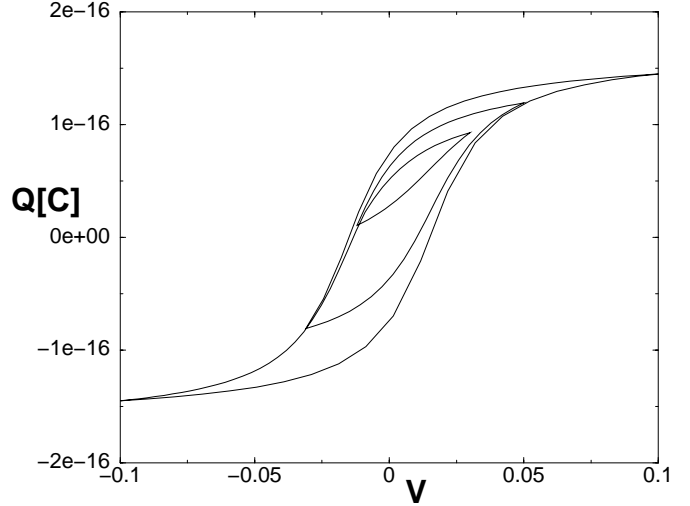

Figure 1: Simulated hysteresis including multiple subcycles

2.1 Hysteresis Model

MINIMOS-NT offers a rigorous approach to treat the static hysteresis properties [2][3] of ferroelectric materials, which was recently extended to the exact calc-Comparison between simulationulation of subcycles.

Using the box integration method, the third Maxwell equation [4]

$$\mathrm{div}\vec{D} = \rho \qquad (1)$$

is solved. To bring in hysteresis, we separate the electric displacement into a linear and a nonlinear part

$$\vec{D} = \epsilon \cdot \vec{E} + \vec{P}. \qquad (2)$$

The nonlinear part $\vec{P}$ holds the hysteresis and is modeled by

$$P = k \cdot f(E \pm E_c, k) + P_{\mathrm{off}}. \qquad (3)$$

The parameters k and P_{off} are necessary for the simulation of the subcycles of the hysteresis, the function f is the shape function for the subcycles, E_c is the coercive field.

By now two different types of shape functions are implemented in the simulator, the tanh and the arctan function. The implementation for the tanh shaped function is

$$P = k \cdot P_{\text{sat}} \cdot \tanh(w \cdot (E \pm E_c)) + P_{\text{off}}. \qquad (4)$$

P_{sat} is the saturation polarization. w is a shape parameter and the same for each locus curve. This function is a good approach for the material properties of $\text{PZT}(\text{Pb}(\text{Zr}, \text{Ti})\text{O}_3)$.

$$P = \frac{2}{\pi} \cdot k \cdot P_{\text{sat}} \cdot \arctan(2 \cdot (E \pm E_c) \cdot \frac{k}{w}) + P_{\text{off}}. \quad (5)$$

is the implementation for the arctan shape function. Again, w is the shape parameter. The arctan function covers the physical properties of $\text{SBT}(\text{SrBi}_2\text{Ta}_2\text{O}_9)$ in a very accurate way. A drawback of this method is that the parameters of the locus curves have to be calculated numerically. This leads on one hand to a slight increase of computation time, on the other hand to some complications with regard to the numerical solution of the problems.

Using these subcycles the whole history of the ferroelectric material is simulated. The necessary parameters are calculated according to Preisach hysteresis [5][6]. This allows the simulation of the following effects:

- Locus curves hit last turning point: This allows the simulation of closed subcycles

- Memory wipe out: A turning point erases all information of previous smaller turning points

A complete set of subcycles is plotted in Fig. 1, showing the simulation results for a planar capacitor.

2.2 Transient Model

According to the concept of our device simulator MINIMOS-NT we tried to find an analytic model based on differential equations instead of an approach based on statistical physics [7] in order to model the transient properties.

We extended a common approach [8] for the frequency dependence of linear dielectric materials. We start with the static, nonlinear equation

$$P = f(E(t)). \qquad (6)$$

Following our approach we add a transient term to the electric field

$$E(t) = E_{\text{stat}} + \tau_{ef} \cdot \frac{dE}{dt} \qquad (7)$$

where E_{stat} is the static component of the electric field and τ a material dependent time constant. The actual electric field is calculated and can be entered into (6), thus forming the first term for the transient equation
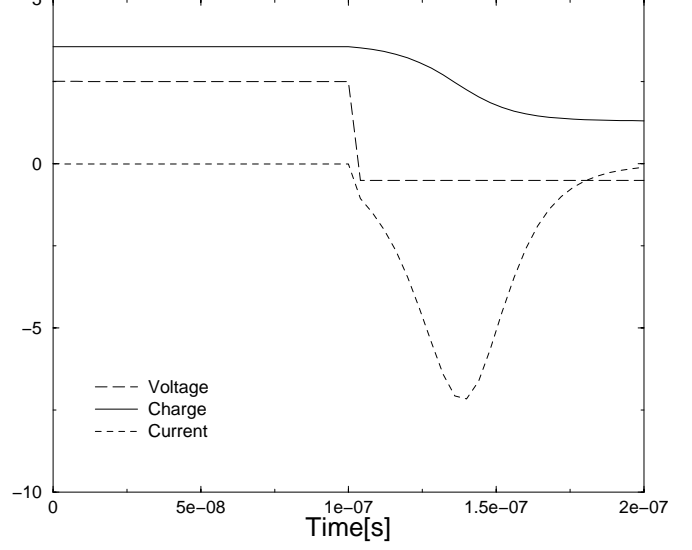
$$P_{\text{ef}} = f(E(t)). \qquad (8)$$

Figure 2: Charge and current response of a voltage jump

Basically, this terms shifts the hysteresis curves and increases the coercive field. Still following the approach for linear materials, we add a transient term stemming from the change of the polarization

$$P_{\text{pol}} = -\tau_{\text{pol}} \cdot \frac{dP}{dt}. \qquad (9)$$

Again τ_{pol} is a time constant. Aside from increasing the coercive field as well, this term flattens the hysteresis. Experimental data shows that these two terms can be fitted into the physical properties in a limited range of frequencies only. In order to improve this,

$$P = P_{\text{pol}} + P_{\text{nonlin}} \qquad (10)$$

a third term, representing the nonlinearity of the material, was added,

$$P_{\text{nonlin}} = c \cdot k_{\text{nonlin}} \cdot (P - P_{\text{ef}}) \cdot \frac{dE(t)}{dt}. \qquad (11)$$

This term allows also a physical interpretation as it increases with the offset between the polarization component stemming from the electric field and the actual polarization. k_{nonlin} is a material dependent constant.

Both transient equations (7) and (10) are discretized with a forward Euler scheme, which garanties a reasonable stability.

3 Examples

With our model, the analysis of ferroelectric memory cells for arbitrary variation of the contact voltage is now possible. Fig. 2 shows the time depending current and charge when a voltage jump is applied to a capacitor, Fig. 3 for a triangular signal with an included delay. Especially in the first of these two figures the behavior
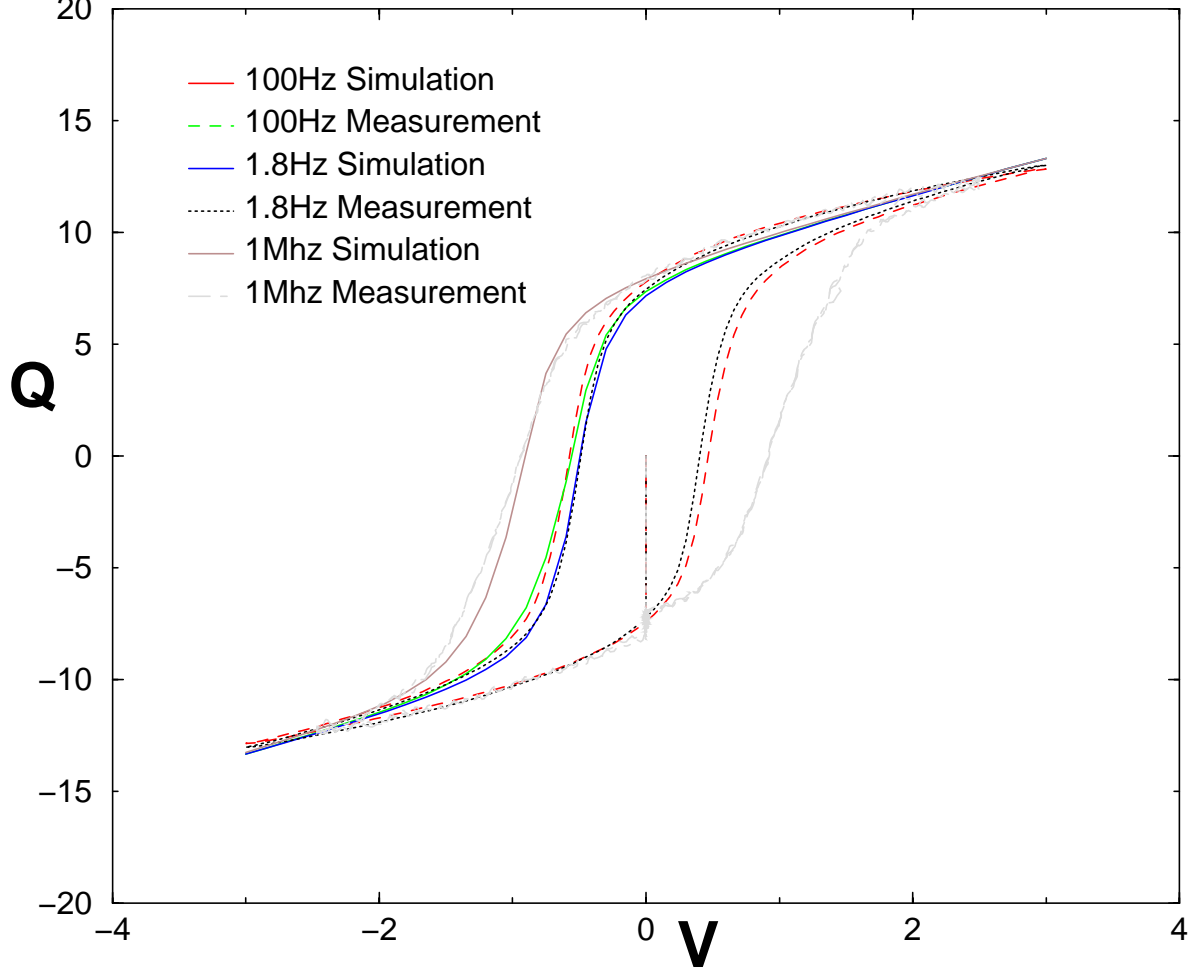
Figure 4: Q/V characteristics - Comparison between simulation and measurement

of the ferroelectric material leads to a significant difference compared with a linear dielectric. The dipole relaxation does not follow an exponential function as might be expected and the maximum current does not appear immediately after the voltage step. As a consequence of equation (7), the electric field cannot change immediately inside the device, so the whole hysteresis curve has to be swept during the relaxation period, which causes the unexpected smoothness of the charge characteristics and the shift of the maximum current to the right.

As outlined above, our model allows the simulation of ferroelectric materials in a wide range of frequencies.

As an example, we have simulated a ferroelectric capacitor in a range beginning from 1Hz up to 1MHz. We extracted the parameters for our model using measurement data following the algorithm outlined in Fig. 5 and a very good fit was achieved (Fig. 4).

From there, frequency dependent material parameters like the coercive voltage (Fig. 6), or the remanent

polarization can be easily obtained. These can be used to emulate the frequency dependence with the static model, which might be useful if the applied frequency stays in the same range.

4 Conclusion

The application of the new simulation tool to circuit simulation is very promising. It can immediately be used for the extraction of specifications for the read and write cycles of ferroelectric memory cells.
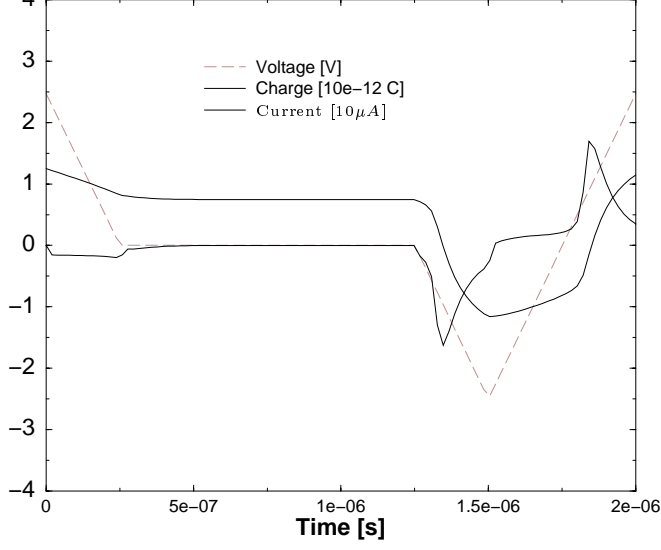
5 Acknowledgement

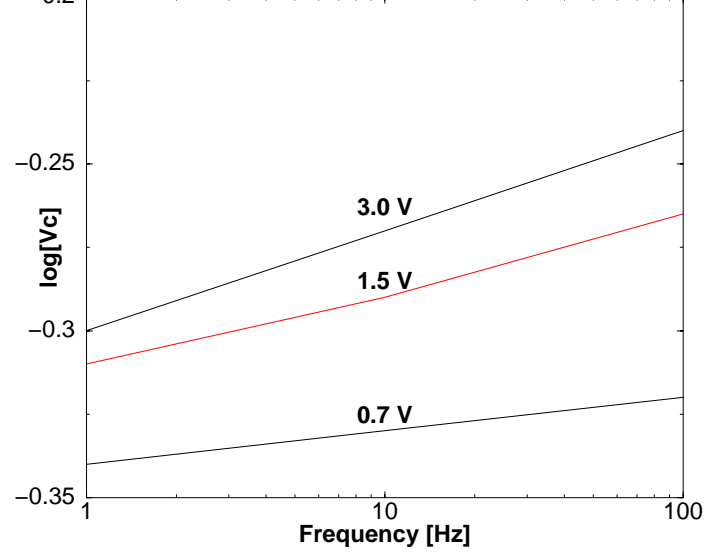Figure 3: Charge and current response of a transient simulation

Figure 6: Coercive voltage as a function of frequency and peak voltage
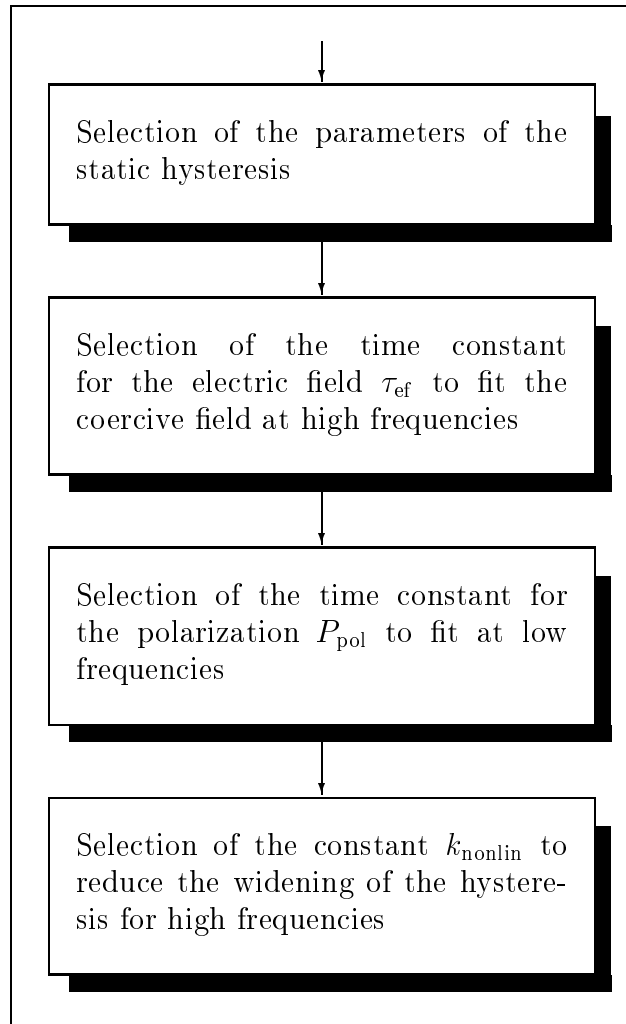

Figure 5: Algorithm to fit the parameters

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