Numerical Aspects of the Simulation of Two-Dimensional Ferroelectric Hysteresis

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ABSTRACT

Simulation of ferroelectric hysteresis allows the analysis of nonvolatile memory cells which are based on ferroelectric materials. We give an overview of our algorithm for the calculation of effects caused by field rotation. Implementation of this algorithm into a device simulator reveals interesting numerical aspects. One of these is that the locus curves of the hysteresis are nonsymmetric, thus demanding a quite sophisticated sign handling to the fields and the fluxes. Another change to common properties is the occurance of history information, which leads to an extension of the discretization. Also the iteration scheme has to be modified, in order to achieve convergence for nontrivial device structures. The abilities of our simulator are demonstrated by the simulation of a ferroelectric memory field effect transistor (FEMFET).

Keywords: hysteresis, ferroelectric materials, FEMFET, nonvolatile memory

INTRODUCTION

The advancing development of nonvolatile memory cells leads to structures which make use of the hysteretic properties of ferroelectric materials. In order to deal with two-dimensional device structures like ferroelectric memory field effect transistors (FEMFET) [1] schematically outlined in Fig. 1, a two-dimensional hysteresis simulator has been developed.

The simulation of the two-dimensional hysteresis curve leads to the nontrivial problem of field rotation [2][3] and requires the calculation of a set of parameters for the non linear locus curves at each grid point. Aside from calculating the exact field distribution a simulator for ferroelectric devices has to fulfill further properties: To allow the calculation of transfer characteristics it has to be insensitive to the magnitude of the applied voltage steps. To keep pace with future developments of ferroelectric devices, the expansion of the algorithm to three dimensions should be possible.

GEOMETRIC ALGORITHM

A general algorithm capable of fulfilling the numerical and physical constraints outlined above was introduced in [4]. It lays special focus on the simulation of field rotation. This enables the calculation of the lag angle χ between the electric field and the dielectric displacement that appears when the direction of the electric field changes.

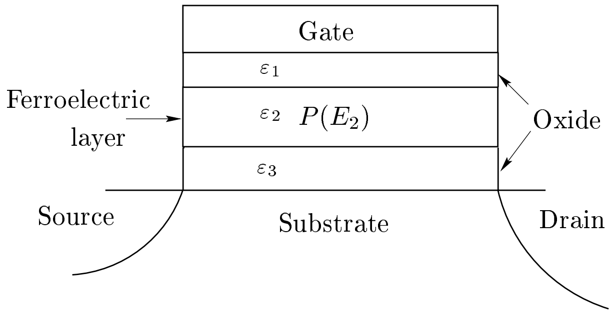

Figure 1: Ferroelectric nonvolatile memory field effect transistor.

The algorithm is based on splitting the polarization vector into orthogonal components with respect to the direction of the electric field at the next operating point. By means of these two components two corresponding locus curves of the hysteresis are calculated, leading to two polarization components, one parallel and one orthogonal to the electric field. These curves yield the polarization in direction of the electric field and some sort of remanent polarization in the orthogonal direction, thus forming a primary guess $\vec{P}_0$ for the next polarization (Fig. 2).

According to the fact that the saturation polarization is forming an upper limit, the component orthogonal to the electric field is reduced if necessary. This leads to the actual polarization vector $\vec{P}_1$ and the lag angle χ and is schematically outlined in Fig. 3.

NUMERICAL PROBLEMS

As a consequence of the general approach, the following numerical aspects have to be considered in order to allow a two-dimensional simulation with the box integration method:

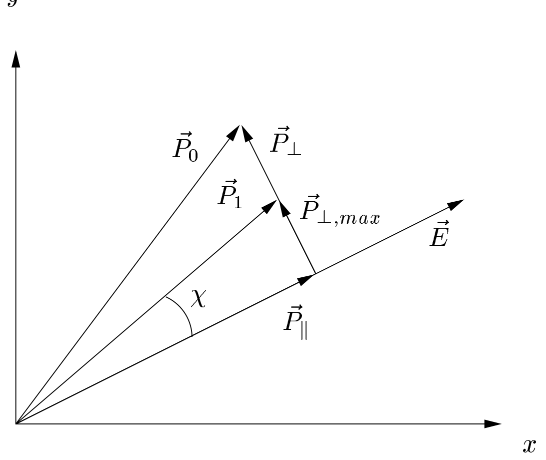

Figure 2: Calculation of the resulting polarization.

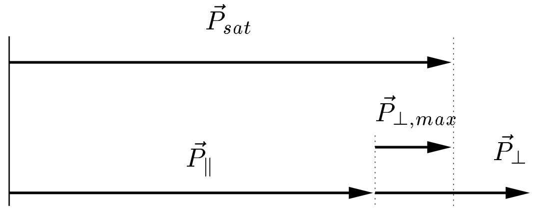

Figure 3: Reduction of the orthogonal component with respect to the saturation.

- Nonsymmetry of the locus curves
- Influence of previous operating points
- Selection of the shape of the hysteresis curve
- Detection of the correct locus curve

Nonsymmetry of the locus curves

In contrast to most of the functions used in device simulation, the locus curves of the hysteresis are nonsymmetric functions of the absolute value of the applied electric field $\|\vec{E}\|$. Different to common properties of symmetric functions, a criterion has to be established which decides whether the argument of the function is treated as positive or negative. Accordingly the orientation of the field compared with the box boundary becomes decisive to the sign of the function argument. Furthermore, it cannot be assumed that the sign of the resulting flux of the electric displacement has the same orientation as the applied electric field.

Influence of the previous operating points

The calculation of the current locus curves uses the parallel and orthogonal component of the previously applied fields in respect to the current electric field. This is a major difference to one-dimensional simulation, which only requires the storage of selected turning points [5]. In order to deal with this information in a suitable way it is necessary to make adjustments to the field discretization. It is intuitive that the history information is required on the box boundary and that it cannot be derived from a representation in the grid points alone, as it is suitable for non hysteretic properties [6].

In case of one-dimensional properties, the orthogonal component has zero length and the parallel component equals the previous electric field, which means that also this special case is covered by the algorithm. In order to speed up the computation the locus curves are not calculated from the last turning point but rather from the saturation polarization, so the lancette curves will not exactly fit the one-dimensional hysteresis model. The resulting locus curves of this approach are plotted in Fig. 4. They were achieved as output of the simulation of a capacitor with ferroelectric dielectric.

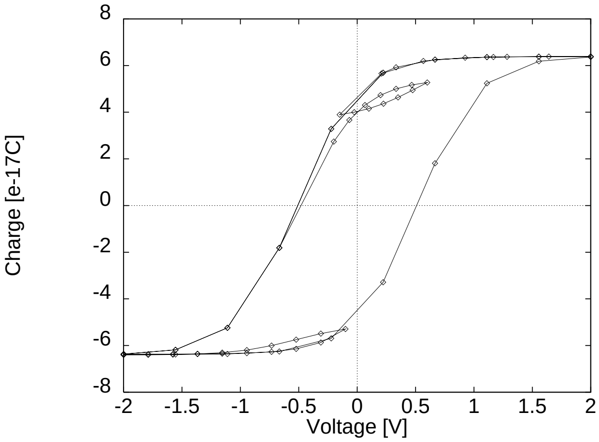

Figure 4: Simulation of a ferroelectric capacitor.

Selection of the shape of the hysteresis curve

Considering the fact that a different locus curve has to be calculated on each box boundary, it is necessary to chose analytic functions. Numerical methods as described in [7] cannot be applied. In order to overcome these difficulties a model was implemented into the device simulator MINIMOS-NT which describes all hysteresis curves by *tanh* functions derived from analytical calculations.

Detection of the locus curve

A sophisticated task is to calculate the locus curves for a new operating point. As outlined in Fig. 5 one of two possible locus curves has to be chosen at each operating point, depending on the history of the electric field [5].

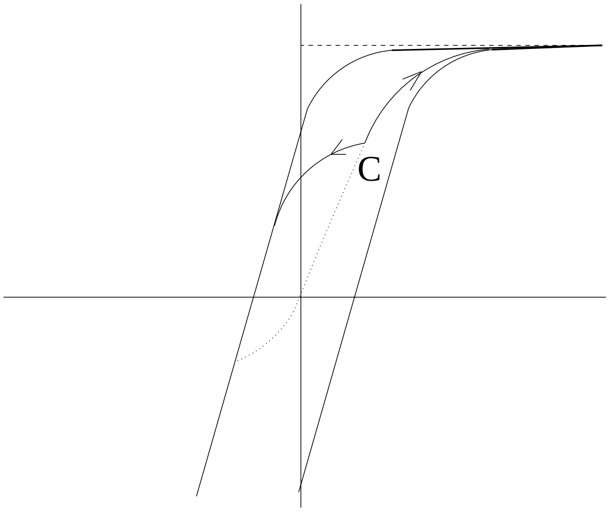

Figure 5: Possible locus curves in an operating point

As a consequence of the two-dimensional algorithm the common starting point C of these two branches will move during the nonlinear iteration. In fact it highly depends on the assumed electric field. Therefore it cannot be guaranteed that the same branch is selected at each iteration step. Regarding the different derivatives of the two functions this will lead to poor convergence and in worst case to oscillations of the nonlinear iteration.

As practice shows a preselection of the correct branch is necessary to achieve convergence, especially for the simulation of complex structures. A suitable approach to detect the direction of the change of the electric field is to solve a linearized equation system. In this system the polarization is kept constant and only the linear part of the dielectric displacement is modified. Using this method an approximation to the electric field in the new operating point is derived.

Based on this information it has to be decided whether the electric field was increased or not. The straightforward approach to compare the absolute values of the old and the new electric field will obviously fail, even if the two field vectors are parallel. For the applied algorithm the parallel component of the old field vector is calculated, and the result is interpreted in dependence of the orientation of the new field vector as outlined in Fig. 6 and Fig. 7.

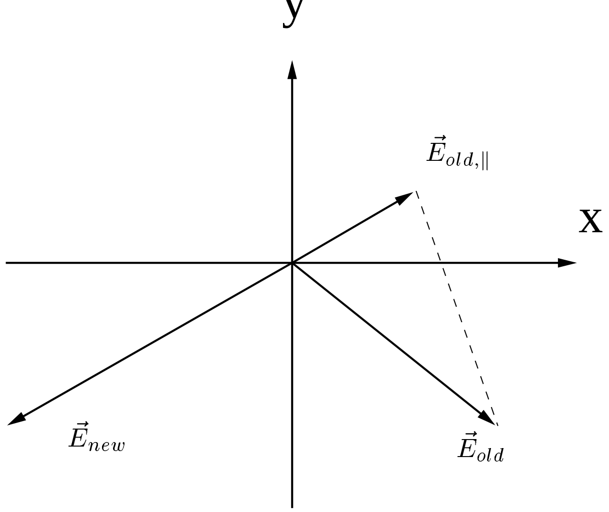

Figure 6: Detection of the change of the electric field, electric field decreases.

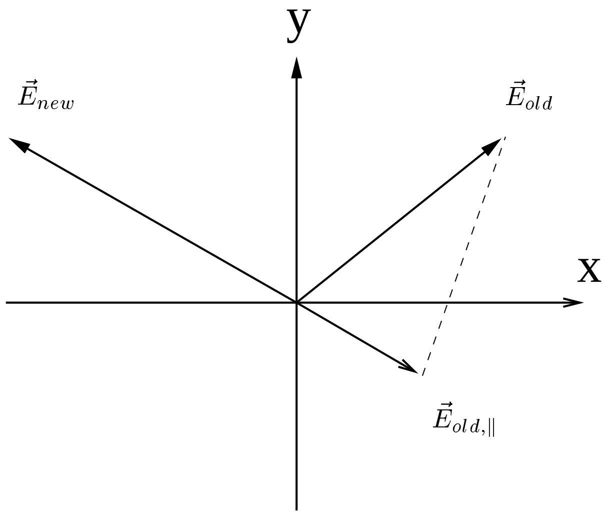

Figure 7: Detection of the change of the electric field, electric field increases.

With this information it is now possible to select the correct branch of the hysteresis curve. The complete scheme is outlined in Fig. 8.

SIMULATION RESULTS

The algorithm was implemented into the device simulator MINIMOS-NT[4]. A FEMFET was constructed by inserting a ferroelectric segment in the sub-gate area of the NMOS, as outlined in Fig. 1. The operating point of the ferroelectric material was chosen on the initial polarization curve. In this case the ferroelectric polarization increases the displacement and leads to a significant higher space charge density in the channel area. This

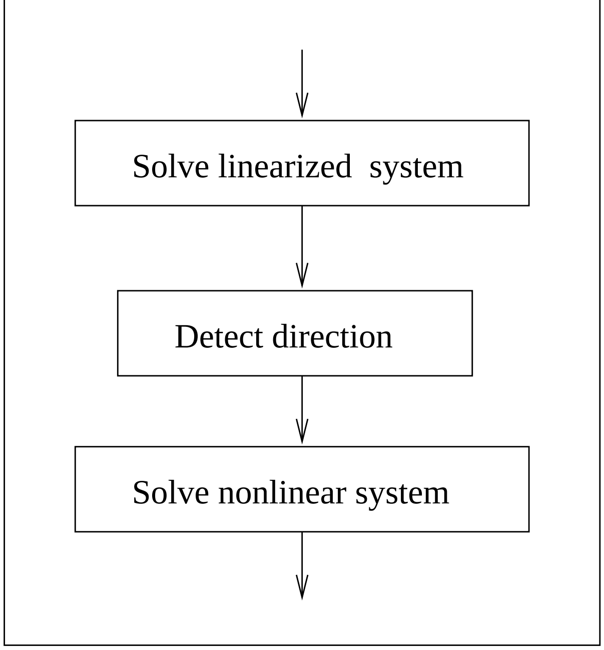

Figure 8: Modified trivial iteration scheme

will cause a higher drain current of the FEMFET for the same gate voltage as for the NMOS. As a result of the hysteretic behavior of the polarization the drain current of the device does not only depend on the gate voltage but also on the history of the gate voltage. So the I–V characteristics of the transistor show also a hysteresis which allows the use of the device as a nonvolatile memory. Fig. 9 sketches the simulated I–V characteristics for NMOS and FEMFET obtained by sweeping the gate voltage from zero to saturation and vice versa The threshold voltage of the NMOS was 0.7 V and 0.6 V for the FEMFET. The bulk voltage was set to 0.5 V, the drain voltage to 0.1 V. We received a voltage shift of 0.1 V. Caused by the higher displacement, the drain current of the FEMFET is significantly increased compared to the NMOS.

CONCLUSION

The implementation of a general two-dimensional algorithm to cope with hysteretic field properties into a device simulator leads to an increase of the numerical effort. We showed that it is possible to implement a two-dimensional algorithm into a device simulator. With calibration of simulations to measurements effective material parameters for the new ferroelectric device technology can be computed.

ACKNOWLEDGMENT

This work is supported by Siemens EZM, Villach, Austria and Siemens AG, Munich, Germany.

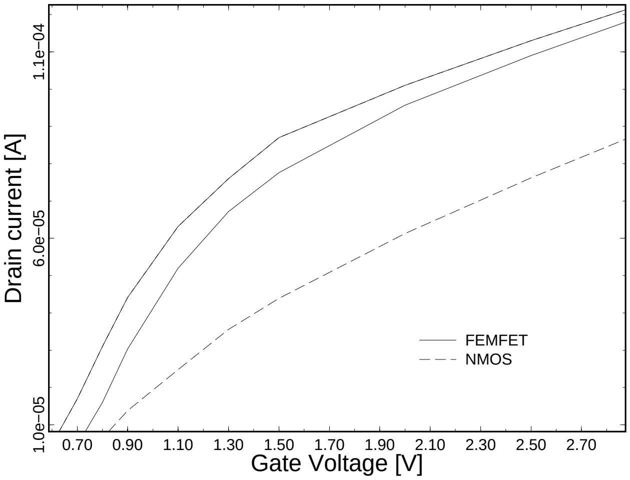

Figure 9: Simulated I-V characteristics of FEMFET and NMOS

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