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SIMULATION OF FERROELECTRIC THIN FILMS

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The hysteresis properties of ferroelectric thin films open an elegant and promising way to build nonvolatile memory cells. Our basic goal is to set up a tool which is able to reproduce the macroscopic behavior of the devices by calculating current, voltage and charge at the contacts correctly. Our tool, MINIMOS-NT, provides a rigorous approach to describe the static hysteresis properties of ferroelectric materials including the accurate modeling of subcycles. Expansion of this model into two dimensions allows the simulation of arbitrary device structures. The generic implementation of our device simulator can handle both isotropic and anisotropic materials respectively. Additionally, we introduced three transient terms with physical meaning into the basic material equation making the simulation in a wide range of frequencies possible.

Keywords: Hysteresis; Two-dimensional simulation; Anisotropy; Ferroelectric materials; Nonvolatile memory

1. INTRODUCTION

During recent years ferroelectric materials have become more and more attractive for usage in nonvolatile memory cells. By now only a few approaches for the simulation of these materials have been tried. Most of them were designed with respect to circuit simulation and provide compact models which allow no insight into the field distributions inside the device [1, 2]. Other approaches analyze the material on particle level [3] and require a high numerical effort. The aim of this work is to close this gap by the

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development and the implementation of a ferroelectric model for the device simulator MINIMOS-NT. The model allows an accurate analysis of devices with arbitrary two-dimensional geometry, and includes the treatment of contact quantities like current and charge and the field distribution as well.

2. SIMULATION MODEL

Simulation of ferroelectric domains and impurities is far from trivial and needs detailed information about the impurity distribution, which is usually not available and specific for a particular device. According to this, the resulting domain structure even differs for devices with identical geometry and identical contact quantities. For our approach we set up the ferroelectric material as a homogeneous cluster of dipoles, each of them showing the macroscopic hysteresis properties. Hysteresis is simulated according to the Preisach model [4]. This includes an exact description 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

Expansion of hysteresis into two dimensions leads to a drastic increase of the complexity in the numerical and physical properties. Especially the effects concerning field rotation demand the development of a two-dimensional algorithm [5]. It has to take into account the remnent polarization components orthogonal to the electric field, respecting the fact that there is an upper limit to the number of dipoles as well. The generic approach implemented in our device simulator MINIMOS-NT can handle both isotropic and anisotropic materials respectively.

Due to our generic approach, our algorithm is capable to deal with materials with one, two or three anisotropic axes with arbitrary orientations. We assume that all dipoles have to be oriented in one of these axes. Turning processes which might occur at high fields are neglected, as the dipoles have to switch between the anisotropic axes. Furthermore we presume that the number of dipoles and domains is still big enough to decrease the field outside of the simulated area to zero.

Simulation of more than one anisotropic axis needs an advanced simulation approach. It has to be considered that the number of dipoles is finite.

This sets a fixed limit to the sum of the polarization components of all axes directions. When this limit is reached the polarization components have to be reduced properly. A good approach is to reduce the components according to the electric field components in the axes directions. Additionally, we introduced three transient terms with physical meaning into the basic material equation. This makes the simulation of frequency dependence in a wide range of frequencies possible [6].

3. SIMULATION OF A THIN FILM

Simulation of a capacitor under consideration of anisotropy leads to remarkable results. Figure 1 shows the different down branches of the hysteresis obtained with the algorithms outlined above for different orientations of the axis of a material with uniaxial anisotropy. The absolute charge in the capacitor decreases with the angle. Furthermore, as a consequence of the geometric properties, the coercive field increases. The non-linearity of the material leads to a nontrivial field distribution, plotted in Figure 2 if a voltage is applied to the capacitor. Due to Poisson's equation, the displace-

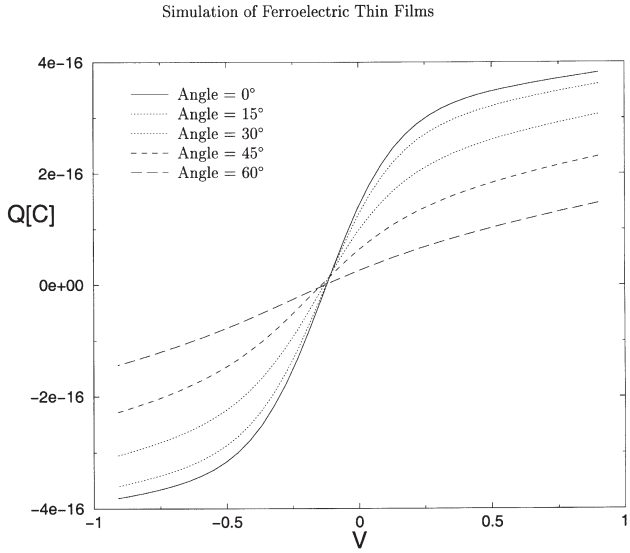

FIGURE 1 Hysteresis curves for different orientations of the axis, uniaxial anisotropy.

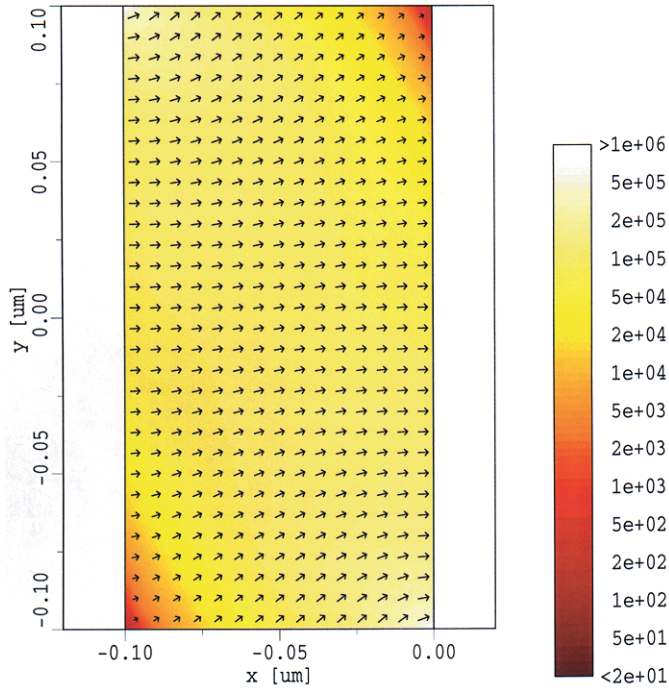

FIGURE 2 Distribution of the electric field, angle = 45°, uniaxial anisotropy.

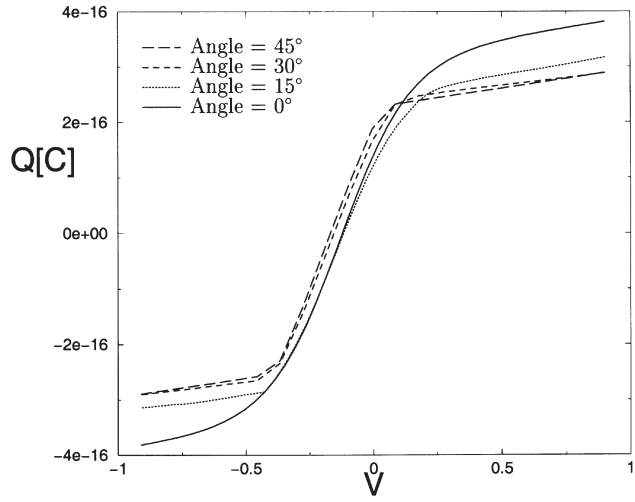

FIGURE 3 Hysteresis curves for different orientations of the axes, biaxial anisotropy.

ment, and as a consequence of the monotonic D/E characteristics the electric field decreases near the charge free boundary. Simulation of a material with two anisotropic axes leads to the resulting Q/V characteristics plotted in Figure 3. The kinds occur when the axial components are reduced because their sum exceeds the saturation polarization.

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 and for the accurate analysis of complex structures as well.

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