I. INTRODUCTION

Ferroelectric material, once electrically polarized, remains polarized even in the absence of an electric field. This is due to hysteresis in the polarization response of the ferroelectric material to electric fields. Two remnant polarizations are available, of opposite polarity but equal magnitude. Data-storage devices with a ferroelectric component make use of these states. The two possible remnant polarizations are related to a logic “0” and “1”, memory states that can be stored without needing a supply voltage or cyclic refreshing. The ferroelectric component can also offer a low programming voltage, radiation hardness, and nondestructive read out. Owing to these properties, ferroelectric memory devices such as ferroelectric random-access memories and on thin-film transistors with a SnO₂:Sb semiconductor and a Pb(Zr,Ti)O₃ ferroelectric insulator can be reproduced and interpreted with the equivalent-circuit models.

II. CHARGE-DISPLACEMENT MODEL

In this section we explain the conceptual origin of our compact model for ferroelectric switching. It starts with the observation that the movement of charge in a material is partly accompanied by energy dissipation and partly dissipationless. For example, the polarization of core electronic states is dissipationless, while the hopping of free carriers or migration of ions involves the dissipation of energy. In a one-dimensional model the dissipationless charge movement is described by a serial arrangement of capacitors [Fig. 1(a)]. Nodal point \( i \) between capacitors \( C_{i+1} \) and \( C_i \) defines the electrostatic potential \( V_i \) at point \( x_i \). The displaced charge per unit area \( Q_i \) displaced in capacitor \( C_i \) depends on the drop of electrostatic potential \( V_i \) .

Dissipative charge transport of particles of species \( s \) (e.g., electrons) is described by a serial arrangement of resistors [Fig. 1(b)]. At the nodal points \( i \) the electrochemical potential \( V_i^s \) of species \( s \) at position \( x_i \) is defined, assuming local thermal equilibrium. The current flowing through resistor \( R_i^s \) depends on the local drop of electrochemical potential \( V_i^s = V_i - V_{i-1} \). The channel for dissipative transport of species \( s \) (\( R_i^s \)) is coupled to the electrostatic backbone (\( C_i \)) when species \( s \) carries electrical charge. The coupling strength—in our model given by \( C_{i}^{DOS,s} \) —is proportional to the local density of states per unit energy [see Fig. 1(c)]. For unit-charge particles \( C_i^{DOS,s} = e^2 \times DOS_s \), where DOS \( s \) is the density of states for species \( s \) (units \( m^{-2} J^{-1} \)).

The equation describing the charge displaced in capacitors and the current flowing through resistors can be a linear as well as nonlinear function of the potentials, depending on...
The physical equations governing the charge movement. If more than one species is being transported, the model consists of parallel channels $s$ that all link to the electrostatic channel (the backbone) at nodal points $i^s$ with DOS capacitors $C^{DOS,s}_i$. In the following section we will explain how these principles can lead to a compact equivalent-circuit model of ferroelectric material.

### III. FERROELECTRIC MODEL

Ferroelectric materials are characterized by bistable charge-displacement characteristics. The bistability is generally caused by off-centered ions in the atomic unit cell each of which can flip from one off-center position to the other when it has sufficient energy to overcome the energy barrier in between the two positions. Thus, in its simplest form, the charge displacement in ferroelectric material involves the dissipative transport of one species of charge (i.e., ions) within the atomic unit cells. In Fig. 2 we propose a system of ferroelectric model units that represent atomic unit cells. The dissipative movement of ionic charge within unit $i$ is modeled by resistor $R_i$. The ions cannot cross the unit-cell boundaries; the interaction with neighboring cells is of an electrostatic nature only, so that the channel of dissipative transport (the serial arrangement of $R_i$s) is interrupted in between the ferroelectric units. The coupling between the movement of ions and the local electrostatic potential is described by capacitors $C^{FE}_i$ and $C^{DOS,ion}_i$. Because of the inability of ions to cross the unit-cell boundaries, we use two of such DOS capacitors for one nodal point $i$ while in Fig. 1 a single capacitor is used. It is a general property of ferroelectric materials that the polarization stabilizes at high applied electric field, so that the DOS capacitors are of a saturating nature. A bistable system is created when the resistors $R_i$ have a strongly nonlinear current–voltage characteristic.

An isolated unit of Fig. 2 allows for parallel transport of charge through the capacitor describing electrostatic charge displacement ($C_i$) and through the serial arrangement of two nonlinear capacitors ($C^{DOS,ion}_i$ and $C^{DOS,ion}_i$) and a nonlinear resistor ($R_i$). This arrangement is summarized in Fig. 3, where $R_i$ is denoted as $R_{FE}$ and $C^{DOS,ion}_i$ and $C^{DOS,ion}_i$ are represented by $C_{FE}$. The voltage across $R_{FE}$ is given by $V_1$, the voltage across $C_{FE}$ by $V_2$. Capacitor $C_i$ is denoted as $C_{diesel}$. This set is summarized by the symbol on the right, a ferroelectric capacitor with voltage drop $V_{FE} = V_1 + V_2$.

Next we will choose functionalities for the three components of the ferroelectric model unit. This choice will involve smooth (analog) charge-displacement and energy-dissipation characteristics, although in principle the polarization states of a single atomic unit cell are discrete. In our model the smooth curves represent the average displacement; this average is the same for time averaging or ensemble averaging. Capacitor $C^{FE}_i$ is a linear dielectric capacitor. We base our choice for the functionality of $R_{FE}$ on the picture of bistable ions flipping at a threshold field. Thus, the switching current through $R_{FE}$ should rapidly increase for $|V_1|$ above a threshold value $V_a$ ($V_a > 0$). As an example, we take

\[ V_{FE} = V_1 + V_2 \]
0 is a normalization parameter. Consequently, the simulated hysteresis loop consists of two loops shifted along the voltage axis by \( V_a \). For smaller values of \( \alpha \), this initial depolarization becomes more pronounced.

These expressions stem from Miller’s model equations of ferroelectric capacitors and their specific form is chosen for mathematical convenience and applicability to the experimental data of Sec. IV. \( Q_{\text{SAT}} \) represents the saturation value of the ferroelectric charge displacement and \( Q_R \) the value at \( V_2 = V_a \). An idealized, square hysteresis loop has \( n \sim 0 \) and \( \alpha = 0 \) with \( V_a \) equal to the coercive voltage and \( Q_R \) to the remnant polarization. For larger values of \( \alpha \), the hysteresis loop deviates from the shape of \( Q_{\text{FE}}(V_2) \) and the apparent coercive voltage and remnant polarization are no longer equal to \( V_a \) and \( Q_R \), respectively. Such deviations also occur when increasing the time needed for measuring one hysteresis loop (so, by decreasing the sweep frequency).

IV. SIMULATION RESULTS

A. Ferroelectric capacitor

In Fig. 4(a) experimental data are shown of a ferroelectric capacitor. Figure 4(b) presents a simulation for the serial arrangement of a nonlinear resistor \( (R_{\text{FE}}) \) and a nonlinear capacitor \( (C_{\text{FE}}) \), neglecting the dielectric contribution \( (C_{\text{dieI}} = 0) \). This is to show that the serial arrangement of these two components gives rise to hysteresis behavior with a nonzero coercive voltage, a nonzero remnant polarization, and to a saturating behavior at high applied voltages. The addition of the dielectric contribution [Fig. 4(c)] reproduces the experimentally observed characteristic. The sharpness of the switching-current onset at \( V_1 = \pm V_a \), described by parameter \( \alpha \), is closely related to the retention of ferroelectric polarization in the absence of an external electric field \( (V_{\text{FE}} = 0) \); low values of \( \alpha \) relate to material that retains its polarization effectively, high values give depolarization in time. This is illustrated in the retention graph of Fig. 5, where the decrease of polarization is shown for our model ferroelectric unit at \( V_{\text{FE}} = 0 \) over 16 time decades.
The influence of $\alpha$ on the $Q(V_{FE})$ graphs is particularly notable for voltage sweeps with an amplitude that is insufficient to drive the ferroelectric polarization into saturation, so-called inner hysteresis loops or subsaturation loops. Figure 6(a) shows a set of experimental $Q-V$ curves including subsaturation loops. The loops have a dissimilar derivative $dQ_{FE}/dV_{FE}$ for given $V_{FE}$ (the experimental observation that this derivative is similar among different subsaturated loops is described for example in Ref. 6). In fact, for simulations with a low value for $\alpha$ and $C_{\text{diel}}=0$ [Fig. 6(b)], the derivative is either that of the outer loop or zero. This is due to the fact that no charge is being displaced when the voltage across $R_{FE}$ is lower than $V_{\alpha}$. When a $C_{\text{diel}}>0$ is added, the zero-derivative sections turn into sections with a (constant) derivative equal to $C_{\text{diel}}$ (not shown). The correspondence with the experimental results, especially in those sections, is improved when two dissimilar model units are combined as can be appreciated from Fig. 6(c) in which two units with a different value of $\alpha$ are combined. Possibly, nonuniformities in the material and effects like domain-wall movement and pinning generate the need for dissimilar model units. The use of two $\alpha$-modules also results in two decay characteristics in the retention graph, one giving rise to fast decay of the polarization ($\alpha=0.2$) and one relating to a more slowly decaying component ($\alpha=0.02$). We note that the data of Teowee and co-workers\textsuperscript{17} for Ti/Pb(Zr,Ti)O$_3$/Pt and Ti/Pb(Zr,Ti)O$_3$/Zn capacitors are similar to the retention simulations of Fig. 6(c). The origin of the complex decay behavior may be the presence of nonuniform fields inside the capacitor (e.g., due to space-charge regions near the interface or due to nonswitching layers) or structural inhomogeneities. The influence of depolarization in time is also seen when the measurement of a hysteresis loop is performed more slowly, resulting in a decrease of the apparent coercive voltage and a decrease of the apparent remnant polarization for decreasing sweep frequencies. This well-known property of ferroelectrics is reproduced by our simulations as well (not shown).

### B. Ferroelectric transistor

We will next describe how a thin-film ferroelectric field-effect transistor, shown in Fig. 7 and described in detail in Ref. 3, can be simulated with a compact equivalent-circuit model such as shown in Fig. 1. We treat the case of small source-drain voltages, so that we only need to derive the equations for charge displacement in the ferroelectric material and the semiconductor layer along the normal of the semiconductor/ferroelectric interface (i.e., along the $x$ axis). For the ferroelectric gate insulator we use the model of Fig. 4(c). A description of the band bending and charge accumulation/depletion in the semiconductor layer of thickness $t$ must satisfy the Poisson equation\textsuperscript{18}

\[
\frac{\partial^2 \Phi}{\partial x^2} = \frac{\rho(x)}{\epsilon}.
\]

$\epsilon \Phi(x) = E_c(x) - E_F$ denotes the position of the conduction band edge ($E_c$) with respect to the Fermi level ($E_F$), $\rho(x)$ the associated charge density, and $\epsilon$ the dielectric constant of the semiconductor. We base our equivalent-circuit description of the $n$-type semiconducting material on the general model of Fig. 1(c). One moving charge species is involved, viz. electrons. No current is flowing in the $x$ direction, so that the resistors in the electrochemical channel can be replaced by shorts. The nodal points $t$ are at zero electrochemical potential, corresponding to the Fermi level of the semiconductor material. This yields the model displayed in Fig. 8(a). Parameter $t$ is the thickness of the thin-film semiconducting layer. As is shown explicitly in the Appendix, the array
solves Poisson’s equation for $N$ equidistant points $x_i$ when we define for $Q_i$ (on $C_i$) and $Q_i^{DOS,e}$ (on $C_i^{DOS,e}$)

$$Q_i = \frac{\varepsilon}{\Delta x} \left[ \Phi(x_i) - \Phi(x_{i-1}) \right],$$

(3a)

$$Q_i^{DOS,e} = -\varepsilon \Delta x \int_{-\infty}^{\infty} f(E)D(E-e\Phi(x_i))dE + q_0,$$

(3b)

with $f(E)$ the Fermi-Dirac distribution function and $D(E)$ the density of electron states (in $m^{-3}J^{-1}$) in the semiconductor. Parameter $q_0$ ensures charge neutrality for zero gate-voltage. Since we are using a degenerately doped semiconductor material\(^{19}\) we choose $q_0$ such that the Fermi level lines up with the conduction band edge at $\Phi=0$. We assumed that the influence of the source-drain voltage on the band bending is negligible, so that we can approximate the source-drain conductivity ($\sigma$) by counting the electrons in states above the conduction band edge ($n_{\text{cond}}$) and calculating $\sigma(x) = n_{\text{cond}}(x) \times e \times \mu$ [see Fig. 8(b)]

$$\sigma(x) = e\mu \int_{e\Phi(x)}^{\infty} f(E)D(E-e\Phi(x))dE,$$

(4)

for $n$-type conduction with electron mobility $\mu$. We assume that the conduction band shape is parabolic, i.e., $D(E) \sim (E - E_c)^{-1/2}$.\(^{20}\) To model the grain boundaries in the polycrystalline semiconductor material a constant density of grain-boundary states ($D_g(E) = D_g$ for all energies) is added to the DOS. Grain-boundary states with an energy inside the semiconductor energy gap are assumed to have zero mobility; states above the gap are assumed to be part of the conduction band. The sheet conductance ($G$) of the transistor finally follows from

$$G = \int_0^l \sigma(x)dx \approx \sum_{i=0}^{N} \sigma(x_i)\Delta x.$$

(5)

This summation is performed by an array of resistors, see Fig. 8(b), each having a conductance equal to $\sigma(x_i)\Delta x$.
of charge into the interfacial layer between the semiconductor and the ferroelectric material.

In panels a3 and b3, the $Q-V_G$ and $I_D-V_G$ curves are combined to a curve of the conductance of the source-drain channel ($G$) versus the charge density displaced in the gate insulator. The slope of the $G-Q$ curve in the high-conductivity (or accumulation) regime determines the electron mobility in the semiconducting channel; the deduced value ($1.3 \times 10^{-4}$ m$^2$/Vs) is in agreement with measurements of the Hall mobility in the same material.\textsuperscript{19} The slope of the $G-Q$ curve at low conductivity (depletion or sub-threshold regime) is given by the density of grain states $D_{gr}$ and the effective semiconductor layer thickness $t_{eff}$. These parameters cannot be deduced independently from the measured curve. However, the semiconductor band bending required for the displacement of a given amount of charge increases for increasing $t_{eff}$, because the band bending in the semiconductor should be smaller than the applied gate voltage minus the voltage required for ferroelectric switching, we can deduce an upper limit for $t_{eff}$ (so also a lower limit for $D_{gr}$). The deduced value is about 2.5 nm, which is of the same order as the Fermi wavelength of the charge carriers\textsuperscript{19} and smaller than the nominal thickness of 10 nm. We attribute this difference to the granular nature of the semiconducting material\textsuperscript{19} and to depletion effects near the semiconductor/capping interface. The fact that several nanometers of the film thickness do not contribute to the conduction is in agreement with our experience that laser-ablated thin films of SnO$_2$ with a nominal thickness below 10 nm show a strongly reduced conductivity compared to films of only slightly larger thickness. The fitted value of the density of grain-boundary states is $8.5 \times 10^7$ F/m$^3$, corresponding to a state density of $1.8 \times 10^{20}$ cm$^{-3}$.\textsuperscript{25} This value is in the expected range for polycrystalline material.\textsuperscript{26,19} Finally, we observe hysteresis in panels a3 and b3 with a clockwise sense of rotation. This is caused by charge trapping in the interfacial layer between the semiconductor and the ferroelectric material. From comparison of experimental and simulation results, no precise value for $C_{trap}$ could be concluded. The similarity between the $G-V_G$-curves for both sweep directions suggests that charge injection into the trapping layer occurs only at high gate voltages. Due to leakage currents in the same regime, it is difficult to estimate values for $V_B$, $I_D$, and $C_{trap}$. Thus, we have chosen them as to yield a sharp transition from zero trapping to complete trapping of all additional charges when $|V_G| \sim 3$ V, indicated for example in panel b3 of Fig. 10.

V. SUMMARY AND DISCUSSION

This article describes a model for the electrical switching characteristics of ferroelectric material in devices such as capacitors and field-effect transistors. The model is based on a compact modeling concept of charge displacement as a function of position in a material, distinguishing dissipative and dissipationless currents. Dissipative transport is described by a channel of resistors; the current that flows...
through the resistors depends on the drop of electrochemical potential inside the material. The dissipationless transport occurs in a channel of capacitors across which a drop of the electrostatic potential is present. The two channels are coupled by capacitors that relate to the local DOS inside the material. The model is used to derive a resistor/capacitor unit that reproduces the ferroelectric switching behavior of an atomic unit cell (Fig. 3). A serial arrangement of a capacitor of saturating nature and a resistor with an exponential current–voltage behavior yields ferroelectric-type charge-displacement characteristics. Important in this model unit is the degree of nonlinearity of the resistor (described by parameter \( \alpha \)) which determines the sharpness of the onset of switching and the time-dependent depolarization of the material. A combination of fast and more slowly decaying polarization components (experimentally observed in Ref. 17 for example) can be simulated by utilizing multiple model units with differing values for \( \alpha \). Good agreement is obtained between experimental characteristics (i.e., charge displacement and transfer characteristics) of ferroelectric thin-film transistors and simulations based on our ferroelectric model combined with a model for the semiconductor and for the ferroelectric/semiconductor interface. The latter two models are derived from the same modeling concept that generated the ferroelectric unit. Charge displacement in the semiconductor channel is calculated along one dimension, sufficient to describe the linear regime of transistor operation \((V_{SD} \ll V_G)\). The model can be straightforwardly extended to describe displacements in two or three dimensions by extending the network of Fig. 1. From the comparison between experiment and our model we conclude that at the most 25% of the nominal 10 nm thickness of the SnO\(_2\):Sb layer (the transistor channel) is conductive. This we attribute to the granularity of and depletion effects in the semiconductor thin film.

In this work we have developed models describing ferroelectric-type, semiconductor-type, and injection-type charge displacement from a single concept model. This model takes into account fundamental material parameters such as the intrinsic DOS, the dielectric behavior, and dissipative charge transport. Therefore, it appears to be a versatile vehicle for modeling a variety of materials. Inhomogeneities in the material call for dissimilar model units to be connected to each other. As an example, several model units placed in a matrix will allow the study of multicell ordering phenomena such as ferroelectric domain wall movement. The existence of inhomogeneities does in principle endanger the compactness of the model. This situation occurs in highly disordered systems where charge transport is determined for example by percolation (the principle of which is a random matrix of dissimilar resistors) or by variable-range hopping. When sufficiently compact units can be defined, as in the case of our ferroelectric devices, compact modeling can be of great importance to simulate the behavior of the devices when embedded in larger electronic circuits, like for example in sensor systems or in memory chips.

**ACKNOWLEDGMENTS**

The authors thank Sjoerd Zinnemers for providing the experimental data discussed in this article and Harry van Esch, Ben Giesbers, and Hans Cillessen for preparing the devices.

**APPENDIX: THE CHARGE-DISPLACEMENT MODEL SOLVING POISSON’S EQUATION**

Referring to Fig. 8, charge conservation yields

\[
\begin{align*}
\left[ \Phi(x_i) - \Phi(x_{i+1}) \right] & \times C_{i+1} + \left[ \Phi(x_i) - \Phi(x_{i-1}) \right] \\
& \times C_i + \Phi(x_i)C_i^{\text{DOS}} = 0.
\end{align*}
\]

(A)

From (3b) we have

\[
\Phi(x_i)C_i^{\text{DOS}} = \rho(x_i)\Delta x
\]

so that

\[
\frac{-\Phi(x_{i-1}) + 2\Phi(x_i) - \Phi(x_{i+1})}{\Delta x^2} = \frac{\rho(x_i)}{C_i}\Delta x.
\]

(C)

Here, the left-hand side corresponds to minus the second derivative of \( \Phi(x) \) at \( x = x_i \). \( C_i \) is defined by Eq. (3a) as \( \varepsilon/\Delta x \) so that Eq. (C) yields a discretization of the Poisson equation, Eq. (2).

1MRS Bull. 21, 7 (1996).
12SPICE=Simulation program with integrated-circuit emphasis; for a recent overview of the history and features of SPICE-based simulation software, see e.g., A. Vladimirescu, The Spice Book (Wiley, New York, 1994).
13A familiar example of a DOS capacitor is the local charge density in a semiconductor conduction band; the formula \( n = n_e \exp(q \phi - \phi_d)/k_BT \) describes how the local charge density depends on the difference between the local electrostatic potential \( \phi \) and the local electrochemical potential \( \phi_d \), the quasi-Fermi level for electrons), for the case that the Fermi level is situated several times \( k_BT \) below the conduction band edge.
Note the sign of the left-hand side of the equation, which differs from what is commonly used, because of our definition of $\Phi(x)$.

The integrals involving $D(E) - (E - E_c)^{-1/2}$ cannot be solved analytically. We have used both an approximation to the integrals valid for $\Phi > k_B T$ and a discrete set of points from a numerical solution in between which the circuit-analysis software interpolates. The results were sufficiently close to each other.

Because subsaturation characteristics of the ferroelectric transistor are not included in the experimental data, the model contains for simplicity only one ferroelectric unit.

$D_{gr}$ is expressed in $F/m^3$ so that $D_{gr}/e$ ($e$ being the electron charge) in $m^{-3} eV^{-1}$. By assuming an energy gap width of 3 eV this is converted into $m^{-3}$. 

