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Dynamic modeling of hysteresis-free negative capacitance in ferroelectric/dielectric stacks under fast pulsed voltage operation

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Motivation

To overcome the fundamental limit of the transistor subthreshold swing of 60 mV/dec at room temperature, the use of negative capacitance (NC) in ferroelectric materials was proposed [1]. Due to the recent discovery of ferroelectricity in CMOS compatible HfO_2 and ZrO_2 based thin films [2,3], the promise of ultra-low power steep-slope devices seems within reach. However, concerns have been raised about switching-speed limitations and unavoidable hysteresis in NC devices [4,5]. Nevertheless, it was shown that NC effects without hysteresis can be observed in fast pulsed voltage measurements on ferroelectric/dielectric capacitors [6], which was recently confirmed using ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ [7,8]. While in these works only the integrated charge after each pulse was studied, here we investigate for the first time if the transient voltage and charge characteristics are also hysteresis-free.

Dynamic NC Circuit Model

Fig. 1 shows the experimental setup for the pulsed charge-voltage measurements as reported in ref. [8], which we simulate dynamically using a simple equivalent circuit model as shown in Fig. 2. Here, V is the output voltage of the pulse generator, I is the current measured across the 50 Ω input resistance of the oscilloscope, $R \approx 350\ \Omega$ is the total series resistance of the setup and the sample, $C_D = 0.163$ nF is the capacitance of the Ta_2O_5 layer, $C_{Fb} = 0.224$ nF is the dielectric background capacitance of the $Hf_{0.5}Zr_{0.5}O_2$ layer, and V_D and V_F are the voltages across the Ta_2O_5 and $Hf_{0.5}Zr_{0.5}O_2$ layer, respectively. The leakage current I_L through the stack was modeled using a simple Fowler-Nordheim approximation as $I_L = k_1(V_D+V_F)^2\exp(-k_2/|V_D+V_F|)$, with $k_1 = 1.85\ \mu A/V^2$ and $k_2 = 11$ V. The capacitor area is $A = 8850\ \mu m^2$, while the thickness of the ferroelectric and dielectric layers are 11.56 nm and 13.5 nm, respectively. The ferroelectric is modeled by a homogeneous Landau approach as $E_F - E_{bias} = 2\alpha P_S + 4\beta P_S^3$, which is shown in Fig. 3, where P_S is the spontaneous polarization, E_F is the field inside the ferroelectric, $E_{bias} = 0.14$ MV/cm, $\alpha = -4.6\cdot10^8$ m/F and $\beta = 9.8\cdot10^9\ m^5/(C^2F)$ as extracted in ref. [8]. The total polarization is $P = P_S + C_{Fb}V_F/A$. Note that there is no inherent hysteresis in this Landau model. As indicated in Fig. 1, there is a charge $\sigma_{IF} \approx -0.15\ C/m^2$ at the interface between Ta_2O_5 and $Hf_{0.5}Zr_{0.5}O_2$, which leads to a stable P_S pointing upwards when $V = 0$, as discussed in Ref. [8].

Results and Discussion

As an input voltage V for the simulations, the measured voltages from ref. [8] were used, which are shown in Fig. 4a) for four different pulse heights. All other dynamic simulation results are color coded to these respective input pulses. Fig. 4b) and 4c) show the simulated transient currents $I(t)$ and charges $Q(t) = dI(t)/dt$, respectively, in comparison to the actual measurement data, which are in very good agreement with only minor deviations during the discharging process. When we look at the simulated V_F in Fig. 4d), we can see that for the smallest applied pulse (grey), V_F always changes in the same direction as Q, indicating $C_F > 0$. However, for the higher applied pulses (red and blue), when V_F approaches 0.8 V, it suddenly changes in the opposite direction as Q, since the ferroelectric enters the NC region of the 'S'-curve in Fig. 3. Only during discharging, C_F enters the positive region again. For the highest applied pulse (green), the ferroelectric enters the second positive capacitance regime while the voltage is still applied and only shortly enters the NC regime during the rising and falling flanks of the applied pulse. Fig. 4e) shows the polarization as a function of time, which always starts and ends in the negative remanent state due to the interfacial charge σ_{IF}. Here, the time frames in which it holds that $C_F < 0$ can be clearly seen. In Fig. 4f) the simulated leakage current is shown, which was fitted to the experimental data. Lastly, in Fig. 5 we compare our simulation results to the integrated maximum, stored and residual charges (Q_C, Q_{rev} and Q_{res}) as reported in ref. [8], which confirms excellent agreement to the experiment. Our results suggest that previous experimental results on NC in $Hf_{0.5}Zr_{0.5}O_2$ under fast pulsed voltage operation are indeed hysteresis-free even in their transient characteristics, which is critical for CMOS compatible NC transistor applications. Further experiments are needed to assess the NC speed limit in $Hf_{0.5}Zr_{0.5}O_2$, which was only limited by the RC delay in our experiments.

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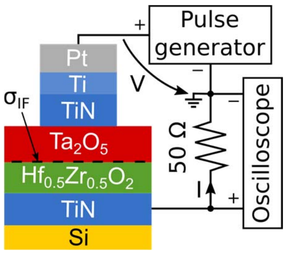

Fig. 1. Sample structure and experimental setup for fast pulsed voltage NC measurements.

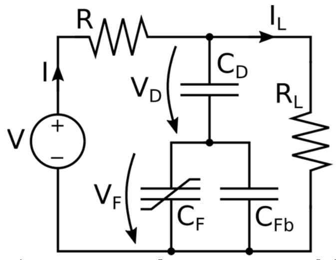

Fig. 2. Equivalent circuit model for dynamic NC simulations of the setup in Fig. 1.

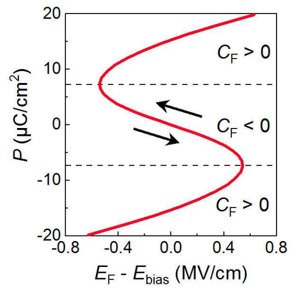

Fig. 3. Landau based ferroelectric model of the $Hf_{0.5}Zr_{0.5}O_2$ layer.

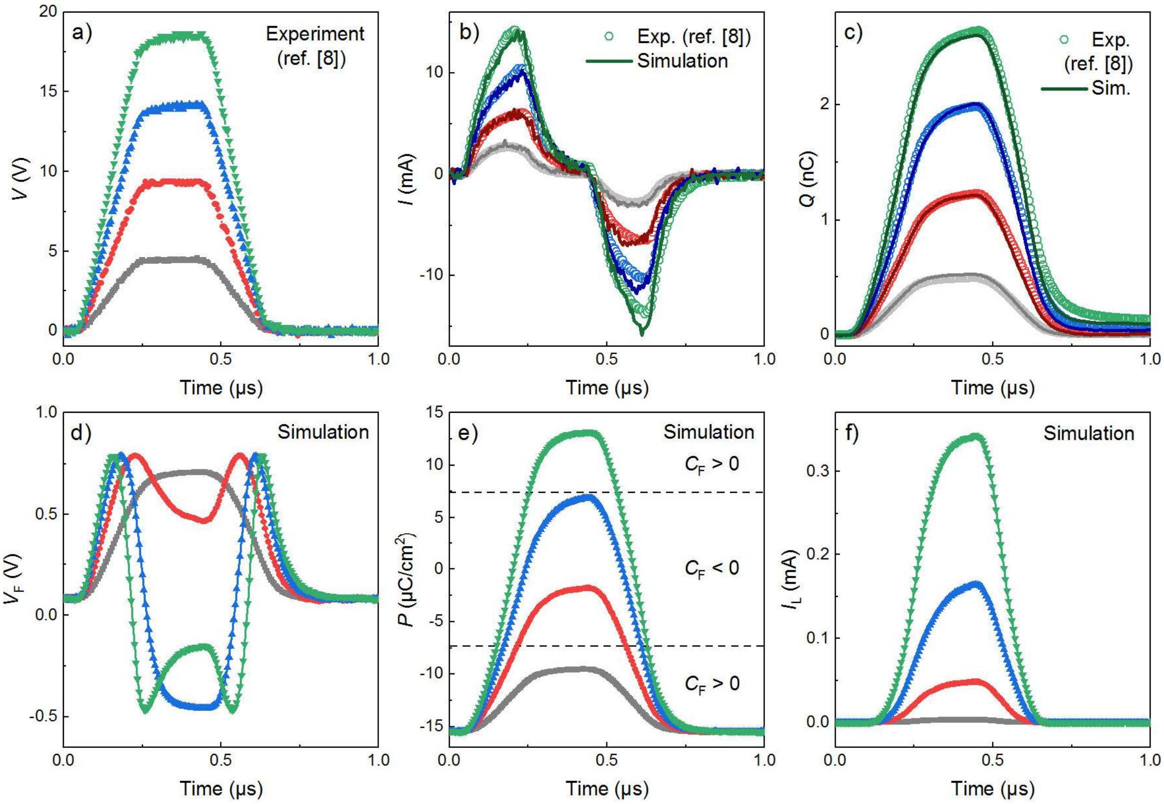

Fig. 4. a) Experimental voltage pulses used for simulation. Comparison of simulated and experimental (Ref. [8]) b) transient currents and c) integrated charges from b). Simulated transient d) voltage across the ferroelectric V_F, e) ferroelectric polarization P, and f) leakage current through the capacitor I_L.

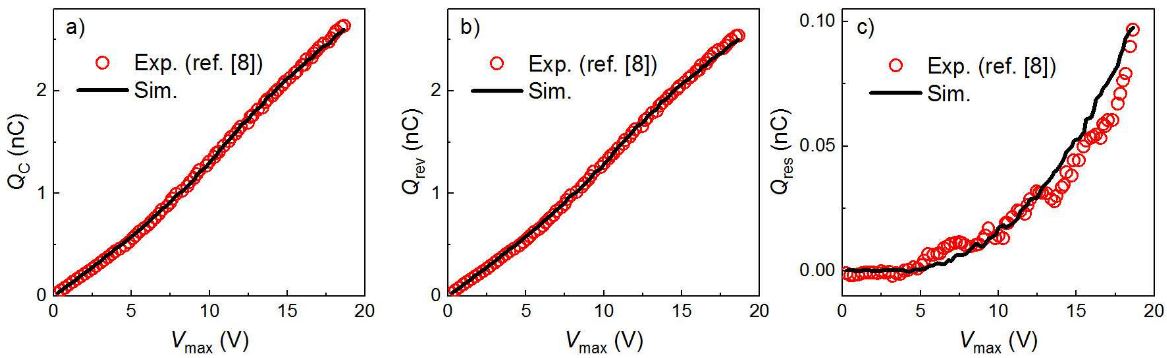

Fig. 5. Comparison of experimental data (Ref. [8]) and simulations of the integrated charges as a function of the maximum pulse height: a) Maximum charge Q_C, b) reversibly stored charge Q_{rev} and c) residual charge Q_{res}.