B. Tech Project Phase 2 Midterm Report

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1 Overview of previous work

In the previous phase pf the project, the work done in [1] was replicated to show the polarization reversal and Polarization-Voltage loops of a poly crystalline ferroelectric. The system considered was made up of multiple grains, with each grain being assigned a activation field E_a which determines the probability of the grain switching at some time t when kept in an electric field E. This probability is given by:

$$P^{(i)}\left(t_S < t+\Delta t \mid t_S > t\right) = 1 - \exp\left[\left(h^{(i)}(t)\right)^{\beta} - \left(h^{(i)}(t+\Delta t)\right)^{\beta}\right]$$

where,

$$h^{(i)}(t) = \int_{t_o}^{t} \frac{dt'}{\tau\left(E_{\mathrm{FE}}\left(t'\right), E_a^{(i)}\right)}$$

$$\tau\left(E_a, E_{FE}\right) = \tau_{\infty} \exp\left[\left(\frac{E_a}{E_{FE}}\right)^{\alpha}\right]$$

The E_a for the grains is determined using a generalised beta distribution of type 2, whose parameters are extracted from experimental analysis. The distribution is given by :

$$GB2(\eta \mid a, b, p, q) = \frac{\frac{|a|}{b}\left(\frac{\pi}{b}\right)^{ap-1}}{B(p,q)\left(1+\left(\frac{\eta}{b}\right)^{a}\right)^{p+q}}$$

The parameters of the distribution taken from [1] are listed below.

Parameter	Value
P_R	$22.9\mu\mathrm{C/cm}^2$
τ_{∞}	387 ns
α	4.11
β	2.07
a	12.1
b	1.79MV/cm
p	0.691
q	0.633

This switching probability was used to build a Montecarlo framework to demonstrate the switching in a ferroelectric. The following results were obtained :

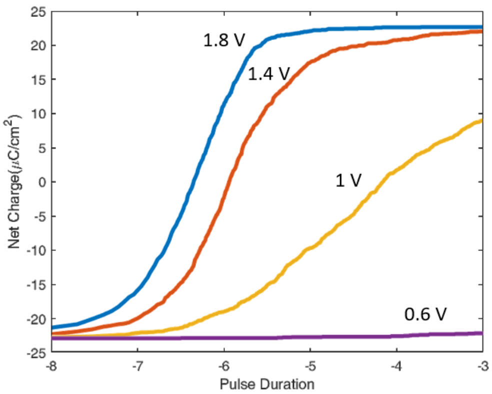

Figure 1: Simulated polarization reversal

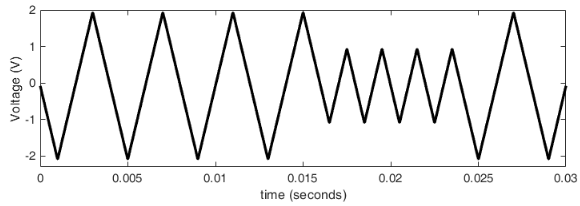

Figure 2: Applied voltage sequence

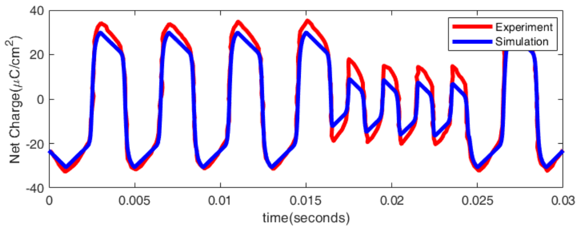

Figure 3: Charge vs time

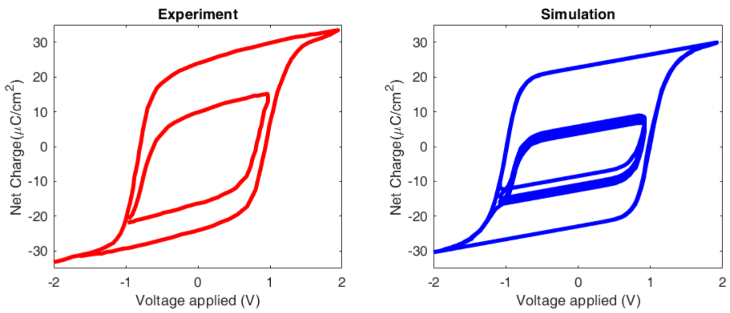

Figure 4: Major and minor Loops seen in hysteresis

2 Present work

In this phase, we have used the model for ferroelectric that we have built in a R-C circuit to demonstrate the transient negative capacitance effect. This effect can be explained by taking a look at the Landau model for single grain ferroelectrics. The Fig. 8 shows the energy vs polarization plot described by the landau equation. The system is initially in one polarization state, and when a electric field of the opposite direction is applied across the ferroelectric, the energy energy landscape changes to energetically favour the other polarization. This causes the system to transition from on well to the other through the energetically unstable negative capacitance state. In order to demonstrate this effect using our monte carlo NLS framework, we consider a

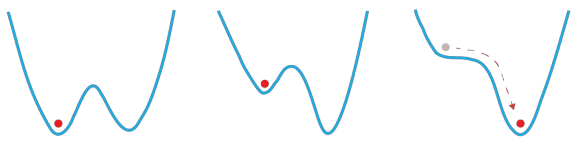

Figure 5: Landau description of transient negative capacitance

RC circuit with the C as our NLS model (Fig. 6). In order to find the voltage across the ferroelectric (V_c), voltage across the resistor (V_R), the charge on the capacitor (Q_c) and the current in the circuit (I), KVL is used :

$$
\begin{aligned}
&V = V_R + V_c \\
&V_R = IR \\
&I = \frac{dQ_c}{dt} = \frac{Q_c(t) - Q_c(t - \Delta t)}{\Delta t} \\
&\Rightarrow V_R = \left[\frac{Q_c(t) - Q_c(t - \Delta t)}{\Delta t}\right] R \\
&V_c = V - V_R \\
\\
&\Rightarrow V_c = V - \left[\frac{Q_c(t) - Q_c(t - \Delta t)}{\Delta t}\right] R
\end{aligned}
$$

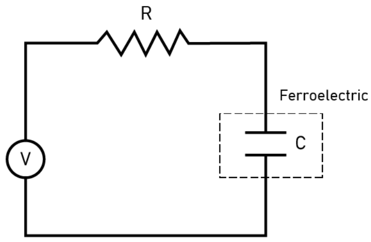

Figure 6: R-C circuit with C being the ferroelectric capacitor

Along with the expression for V_c, we have the NLS model which gives Q_c as a function of V_c. Using these two, we build a iterative loop to obtain Q_c, V_c and I. We apply a step voltage to the system to see the transient behaviour of the capacitor. The circuit is simulated using an iteration loop as shown in Fig. 7.

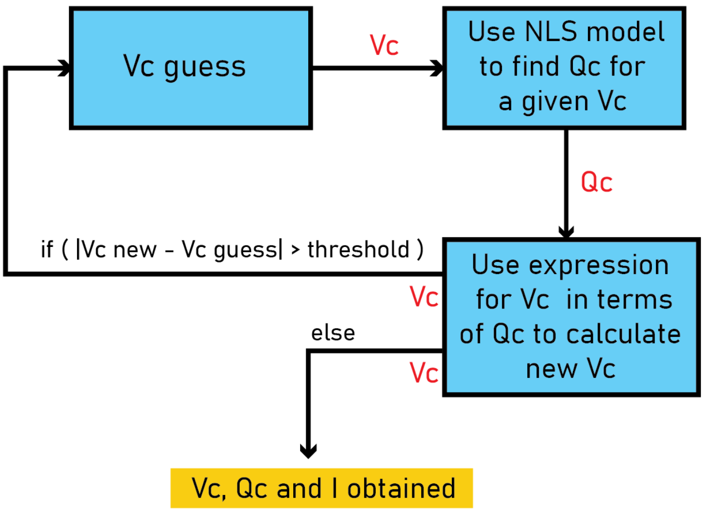

Figure 7: Iteration loop for the RC circuit simulation

The results from the simulation are presented below.

NOTE : The y axis values in these plots are very small as the sample size of the ferroelectric considered is small $((100nm)^2)$*. This was done to reduce the computational load.*

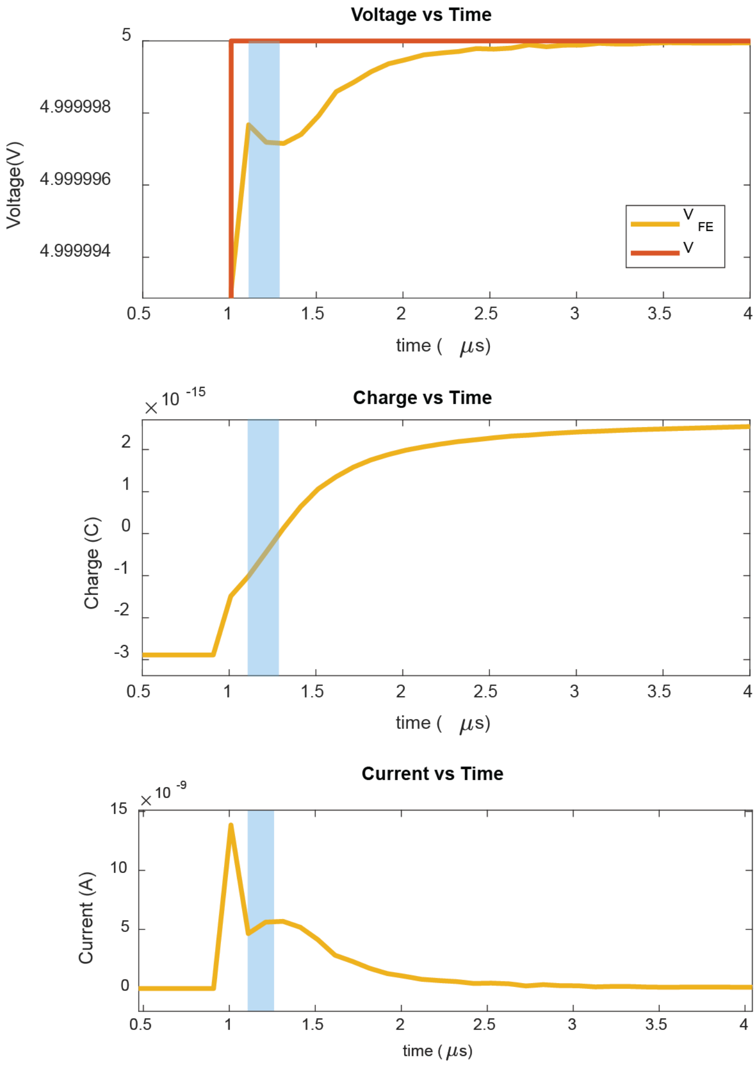

Figure 8: Top: The applied voltage and the voltage across the ferroelectric. Bottom: Charge on the capacitor vs time

It can be seen that there is a brief region (highlighted in blue) where the charge on the capacitor increases as the voltage decreases. This is evidence of transient negative capacitance. This matches the experimental evidence presented in [2]. The plots from this paper are shown in Fig. 9.

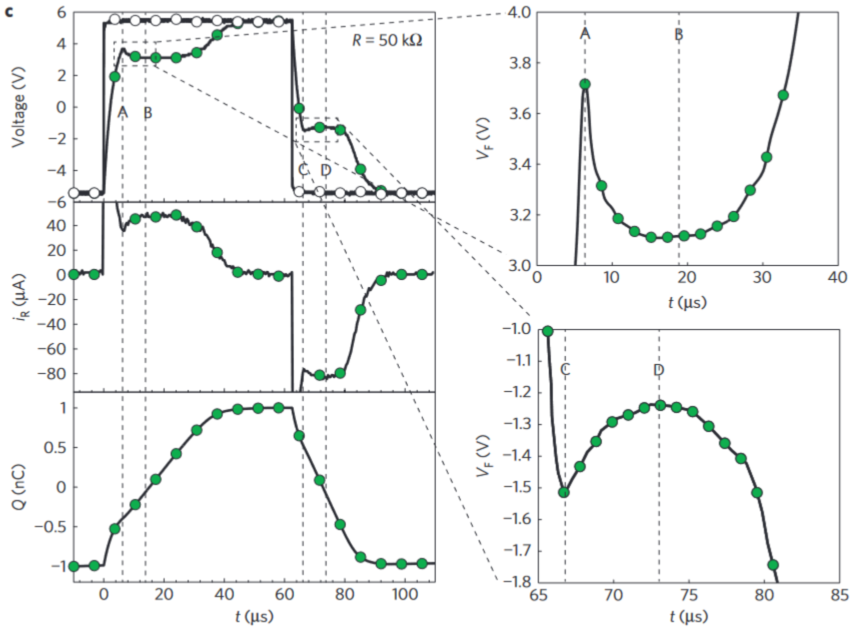

Figure 9: Experimental results showing charge, current and voltage in the circuit. From [2]

3 Future plans

We are currently looking at the analogy between a ferroelectric and a ferromagnet. We expect to see similar behaviour owing to the similaity of the equations when the dual of the series RC circuit is considered, which is a parallel RL circuit. We first will be looking at a single domain ferromagnet and showing transient negative inductance using the landau framework. We then will look at the ising model to model a polycrystalline ferromagnet. This will be accompanied by attempting to experimentally measure the transient negative inductance effect.

References

[1] C. Alessandri, P. Pandey, A. Abusleme, and A. Seabaugh, "Monte carlo simulation of switching dynamics in polycrystalline ferroelectric capacitors," *IEEE Transactions on Electron Devices*, 2018.

[2] A. I. Khan, K. Chatterjee, B. Wang, S. Drapcho, L. You, C. Serrao, S. R. Bakaul, R. Ramesh, and S. Salahuddin, "Negative capacitance in a ferroelectric capacitor," *Nature Letters*, 2014.