B. Tech Project Final Report

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1 Introduction

Ferroelectrics are a class of material that have non-zero net polarization when no external electric field is applied. These class of material have become increasingly important in the recent years with their newfound application in improving transistor performance by reducing the sub-threshold swing and short channel effects. The discovery of ferroelectricity in CMOS compatible doped Hafnia in 2011 [1] has further increased the importance ferroelectrics hold in making the next generation of devices.

Although ferroelectrics have been studied for many years, the origin and behaviour of negative capacitance in ferroelectrics, the effect which allows for the enhanced performance of transistors, is still not well understood. Multiple attempts have been made to understand, model and properly utilize this negative capacitance state, the landau theory being one of the powerful frameworks. In this work, we have used the nucleation limited switching (NLS) mechanism along with a Monte Carlo algorithm to model the behaviour of ferroelectrics. The model described in [2] is recreated and the results presented. All plots shown are simulated using the model built unless stated otherwise.

2 Model Description

The NLS theory says that the ferroelectric has multiple grains that each switch independently of the other when an electric field is applied. The below image illustrates the switching of a FE under an applied electric field. The simulation uses 1000 of these grains(black bordered region) for the results.

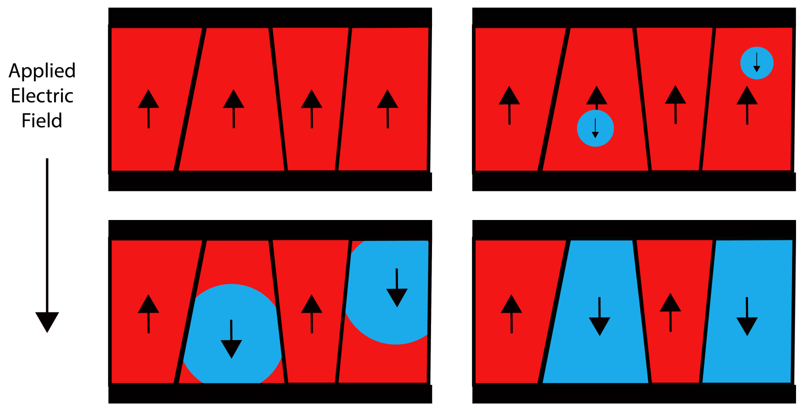

Figure 1: NLS switching

The next subsection provides a mathematical formulation for this switching.

2.1 Theory

(same as what is described in the midterm report)
The original NLS theory [3] says that the nucleation events occur at a constant rate of $\frac{1}{\tau}$. But according to the classical nucleation theory [4], domain nucleation takes place in stages. Based on experimental results[4], the switching can be described as a Weibull process where the CDF of a grain switching before time t is given as :

$$P(t_s < t|\tau, \beta) = 1 - exp\left(-\left(\frac{t}{\tau}\right)^{\beta}\right) \tag{1}$$

This gives a us the time dependent switching rate as:

$$r(t) = \frac{\beta}{\tau}\left(\frac{t}{\tau}\right)^{\beta-1} \tag{2}$$

The tendency of a certain grain to switch is dependent on the activation field of that grain. A probability density function for the activation field for the different grains are obtained through experiments [5]. The pdf follows a generalized beta distribution of type 2 :

$$GB2(\eta \mid a, b, p, q) = \frac{\frac{|a|}{b}\left(\frac{\pi}{b}\right)^{ap-1}}{B(p,q)\left(1+\left(\frac{\eta}{b}\right)^{a}\right)^{p+q}} \tag{3}$$

The time constants τ for the different grains depends on the activation field and the applied electric field as:

$$\tau\left(E_a, E\right)=\tau_{\infty} \exp \left[\left(\frac{E_a}{E}\right)^\alpha\right] \tag{4}$$

The expectation value of equ(1) gives the value of polarization at some time t for a given applied electric field E_{FE} for a system fully polarised to $-P_S$:

$$P\left(E_{\mathrm{FE}}, t\right)=-P_S+2 P_S \int_0^{\infty} P\left(t_S<t \mid \tau\left(E_a, \eta E_{\mathrm{FE}}\right), \beta\right) f(\eta) d \eta \tag{5}$$

Now, we apply this theory to build a Monte Carlo framework. The parameters extracted from experiment is shown in the below table.

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

2.2 Monte Carlo framework

We consider the system to be a set of N grains. Each one is initialized with an activation field E_a using the PDF given in equ 3. Each of grains are given a state $= \pm 1$ depicting upward or downward polarization. The probability of switching for the monte carlo framework for a constant rate constant is given in discrete time as:

$$P^{(i)}\left(t_S<t+\Delta t \mid t_S>t\right)=1-\exp \left[\left(\frac{t}{\tau^{(i)}}\right)^\beta-\left(\frac{t+\Delta t}{\tau^{(i)}}\right)^\beta\right] \tag{6}$$

Foe each grain, this probability is evaluated and switched with the obtained probability. The total polarization of the system is given by:

$$P_{FE}(t)=\frac{P_S}{N} \sum_{i=1}^N s^{(i)}(t) \tag{7}$$

For the non-constant τ case, the term $\frac{t}{\tau}$ is replaced with a history term h defined as:

$$h^{(i)}(t)=\int_{t_o}^t \frac{d t^{\prime}}{\tau\left(E_{\mathrm{FE}}\left(t^{\prime}\right), E_a^{(i)}\right)} \tag{8}$$

The corresponding switching rate is given as :

$$r^{(i)}(t)=\frac{\beta}{\tau^{(i)}(t)}\left(h^{(i)}(t)\right)^{\beta-1} \tag{9}$$

which gives the switching probability :

$$P^{(i)}\left(t_S<t+\Delta t \mid t_S>t\right)=1-\exp \left[\left(h^{(i)}(t)\right)^\beta-\left(h^{(i)}(t+\Delta t)\right)^\beta\right] \tag{10}$$

2.3 Generating random numbers

This model requires generating random numbers according to the generalized beta function of type 2 probability density function. Since this is not a commonly used pdf that is readily available as MATLAB function, we use the inverse sampling method to generate random numbers according to this distribution. Below is the description of this method.

The pdf of the beta type 2 function is given as:

$$GB2(\eta \mid a, b, p, q)=\frac{(|a| / b)(\eta / b)^{a p-1}}{B(p, q)\left[1+(\eta / b)^a\right]^{p+q}} \tag{11}$$

Where B(p,q) is the beta function, η is the variable (activation energy E_a in our case) and a,b,p,q are values obtained experimentally. We now obtain the CDF of the GB2 function. Given by

$$CGB2(\eta) = \int_0^\eta GB2(\eta)d\eta \tag{12}$$

Then, the inverse of the cdf is taken.

$$ICGB2(c) = CGB2^{-1}(\eta) \tag{13}$$

Now, if we input values into the ICGB2 according to a uniform distribution, the function will output values according to the generalized beta function of type two. The proof of this method is explained in []. Below is the histogram of the generated random variables. Each bin is of width of approximately 8e4 V/m (Ea values are the random values generated).

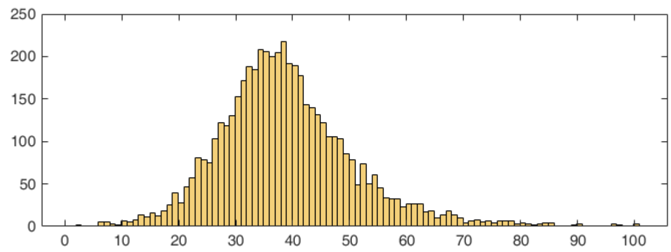

Figure 2: Histogram of random activation field (E_a) values generated using the inverse sampling method

3 Results

All results are obtained with the grain number set as 1000.

3.1 Polarization Reversal

Here, a step voltage pulse of varying duration and voltage is provided to see the transient behavior of the polarization switching. The simulated results (Fig. 4) can be seen to be matching the experimental data.

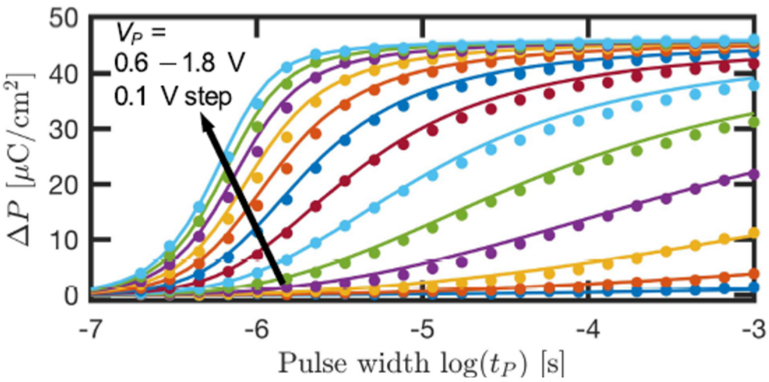

Figure 3: Polarization reversal experimental result (taken from [2])

3.2 P-V Loops

These results illustrate the capability of the model to closely match the experimental data for an arbitrary voltage sequence. The applied voltage pulse is shown in Fig. 5. The corresponding charge vs time plot can be seen in Fig. 6 which shows the experimental data and the simulated result. The charge is then plotted against the voltage applied and Fig. 8 clearly shows the major and minor loops indicating that the model shows the partial polarization behavior of ferroelectrics when a voltage lesser than the coercive voltage is applied.

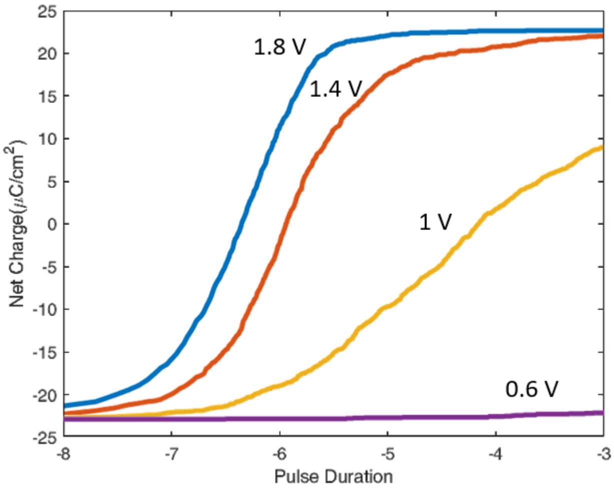

Figure 4: Simulated polarization reversal

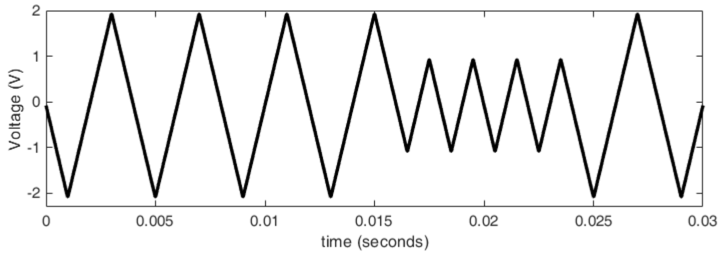

Figure 5: Applied voltage sequence

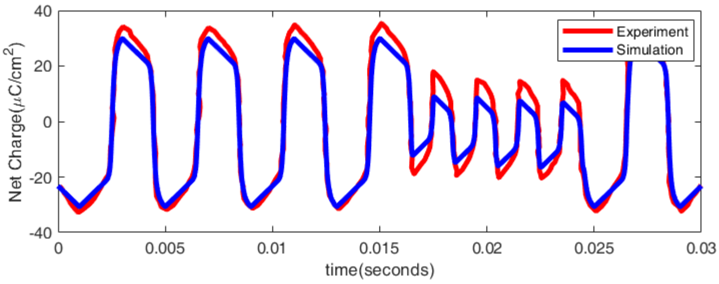

Figure 6: Charge vs time

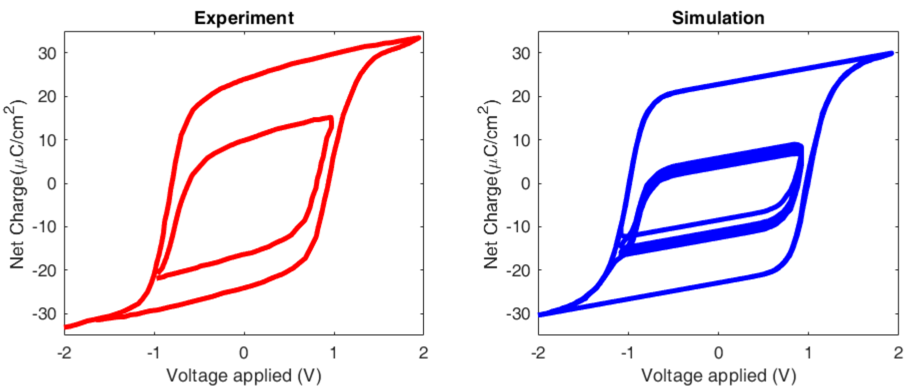

Figure 7: Major and minor Loops seen in hysteresis

Below are the simulated plots given in the paper. The model closely matches the simulated results in the paper.

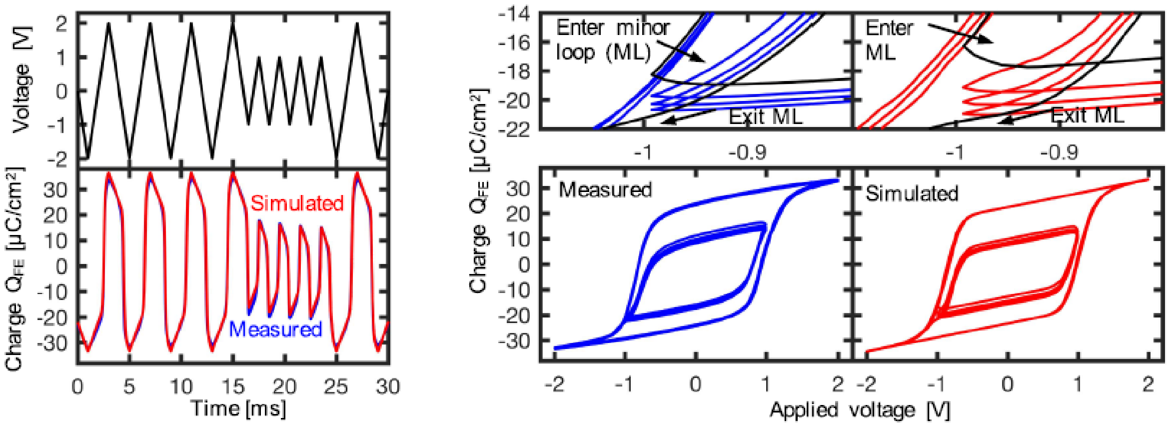

Figure 8: Simulated results from the paper [2]

4 Plan for the next phase

We have obtained the results describing the transient and steady state behaviour of a ferroelectric in response to an arbitrary applied electric field using the Monte Carlo NLS model. Now, we plan on looking at the behavior of a FE-DE stack in response to an applied electric field and correlating it with the experimental results provided in [6]. With this, we expect to see the charge boost effect seen in a FE-DE stack that is stabilised in the negative capacitance state.

References

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