B.Tech Project

Midterm Report

EE4110

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Project title as listed in initial proposal: *Ab-Initio Simulation of Ferroelectrics*

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. This work aims to give a model that predicts the behaviour of ferroelectrics under an applied electric field and allows for researchers to better understand characteristics of ferroelectrics and design devices accordingly.

Our goal in this BTP is to analyse and predict what a ferroelectric would look like in this negative capacitance state, i.e. the polarization orientation of all regions in the FE. We intend to do this with a two scale approach. The first level being looking at the ferroelectric at a microscopic level and understanding the interaction between lattice sites through ab-initio calculations. Next, we use these results to help model the macroscopic behaviour using an Ising model and a monte carlo simulation framework.

2 Progress so far

Before going into ab-initio calculations, we look at the work done in [2]. Here, instead of using ab-initio calculations, they use experimental results to extract parameters required to build a monte carlo model. We have attempted to replicate this model.

2.1 Theory

This work considers polycrystalline ferroelectrics. The system consists of multiple grains that switch independently when a electric field is applied. It uses Nucleation Limited Switching (NLS) theory to obtain the probability of a grain switching. The NLS theory says that a certain grain switches when a region of reversed polarization is nucleated. Once nucleated, the region expands quickly to switch the entire grain. The time taken for this expansion is much smaller compared to the time it takes for the first nucleation event to occur. 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 differnt 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 $-P_S$:

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

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 = ± 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:

$$h^{(i)}(t) = \int_{t_o}^{t} \frac{dt'}{\tau\left(E_{\mathrm{FE}}\left(t'\right), E_a^{(i)}\right)} \tag{8}$$

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 :

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

This framework can now be used for any arbitrary applied electric field waveform. As a first step, we have attempted to replicate Fig.3 in [2] (Shown in Fig.2 for reference). The applied electric field and the result of our simulation is shown in Fig. 3.

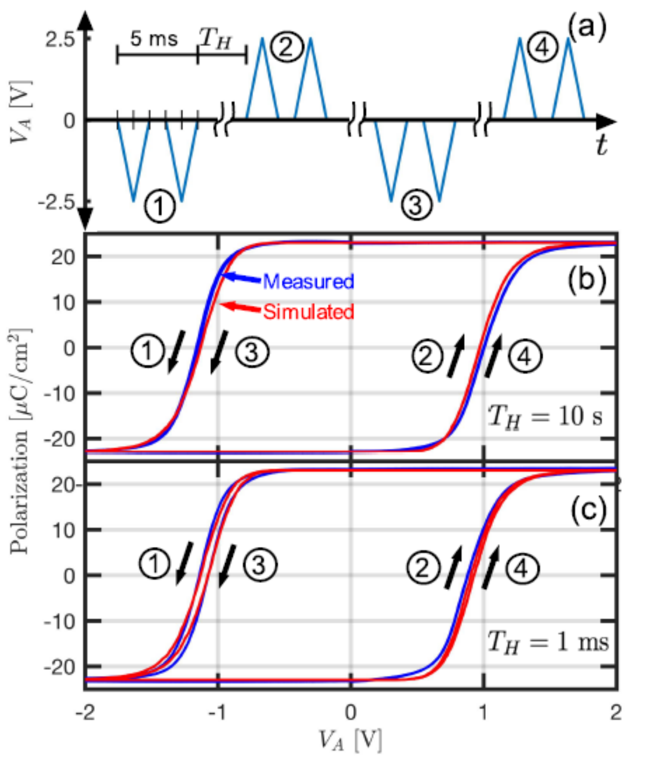

Fig. 3. (a) Experimental protocol to measure *P*–*V* loops. A double triangular waveform V_A is applied. The first triangle produces a current due to the linear capacitance and the polarization reversal. The displacement current due to the linear capacitance alone is measured by the second triangle, where there is no polarization current. A hold time T_H is applied between polarization pulses. Measured and simulated *P*–*V* loops with (b) 10-s hold time and (c) 1-ms hold time.

Figure 1: Image from [2] for reference

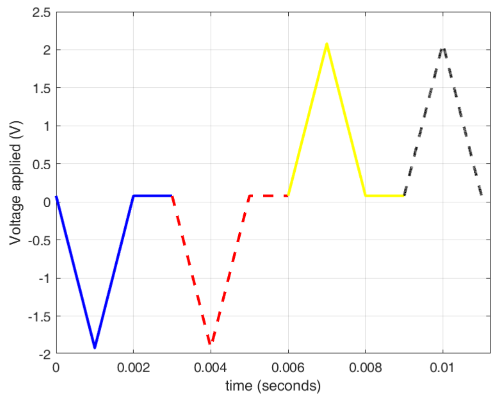

Figure 2: Image from [2] for reference

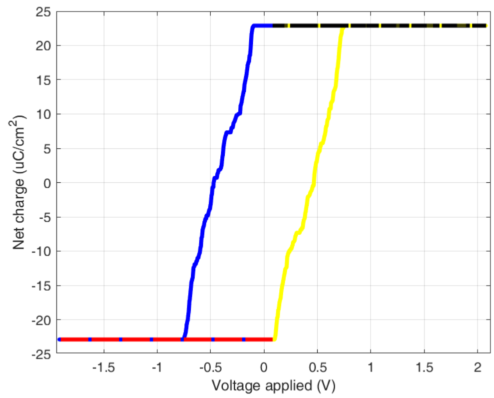

Figure 3: Image from [2] for reference

3 Conclusion

We have performed a literature survey to understand the progress in this area so far. As a first step to understanding modelling using a monte carlo framework, we have attempted to understand and replicate the work done in [2].

References

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