Domain Switching as the Ferroelectric Tester Sees It

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Summary

Nothing electrical can move inside the volume of a capacitor without an electron moving into or out of that capacitor from an external circuit. Those external electrons are the ones that ferroelectric testers keep track of during a test and each one has a story to tell. This is their story.
A ferroelectric capacitor is a 2-port system.
Contents

a) What does a tester see?

b) What is inside the ferroelectric hysteresis loop?

c) Ferroelectric capacitors in a circuit

d) Questions:
   1. KAI vs NLS vs RC?
   2. Nucleation when cold?
   3. Coercive Voltage Stability?
   4. Vortice annihilation everywhere?
   5. Partial Switching?
Balance of Forces

Imagine a perfect capacitor whose two plates are shorted by a perfect wire. Net movement of mass in the circuit is zero. In this condition, the integral of force around the circuit is zero.

Since Electric Field equals *Newtons per Coulomb*, the electric field integrated around the circuit is zero. The sum of forces around the circuit averages to zero even if there may be charged particles here and there.
Return to Zero

Starting from steady state with zero motion, if any charge anywhere inside the capacitor changes its position or its orientation, the sum of electrical forces will not be zero. Charges will move around the circuit to bring those forces back to zero.
The Ferroelectric Tester

A Radiant tester simply sits in the circuit path and counts the electrons going by each way. That count is plotted versus time.

Note: the comings and goings of charge at zero volts is how the Deep Level Transient Spectroscopy (DLTS) Task works.
The Ferroelectric Tester

Adding a voltage source to the circuit simply forces charges to move.

That count over a full voltage cycle is the hysteresis loop.
The Ferroelectric Tester

In summary, a ferroelectric tester will report *everything* that happens inside the capacitor above the resolution of the instrument. In Radiant’s case, that limit is a few 10’s of femtocoulombs.

![Diagram of the Ferroelectric Tester]

- **Tester**
  - Count = 1 at time = 0.1 sec
  - Voltage is optional.
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The Components

• According to Joe:
  – Linear capacitance
  – Non-linear capacitance
  – Remanent polarization

  \[\text{Ignore for now}\]

  – Remanent and non-remanent leakage
  – Remanent and non-remanent small signal capacitance
  – Reverse bias diode electrode interfaces
  – Left-overs
Normalized CV

The normalized CV \([nCV]\) is the mathematical derivative of the polarization hysteresis loop. It has the formula

\[
\frac{\delta P}{\delta V} \Rightarrow \frac{\delta Q}{\delta V} / \text{Area}
\]

and has the units of

\[\mu F/cm^2\]

when the derivation is performed on the polarization units of

\[\mu C/cm^2\]

*It is the Large Signal Instantaneous Capacitance of the sample.*
• C is a constant slope so the derivative of linear capacitance is simply a vertical offset on the nCV plot.
Non-linear Capacitance

This device has both linear and non-linear capacitance. The linear capacitance is the vertical offset of the nCV plot. The tips do not touch zero.
Remanent Hysteresis

Switching and Non-switching half loops:
Remanent Hysteresis

- PUND: $P^r - P^{\wedge}r = dP = Q_{\text{switched}}$
- Hysteresis: Switching - Non-switching = Remanence:
- The nCV of the remanent polarization loop rests on the X-axis because it has no capacitance on the re-trace.
Resistive Leakage in the Hysteresis Loop

- Pure resistance is a “football”.
- The derivative of pure resistive leakage is an “X”.
Is this Ferroelectric?

- Yes, it is ferroelectric! See the ferroelectric remanent polarization switching peaks sticking out of the resistor “X”.

Ferroelectric Capacitor || Linear Resistor
[Test Period = 2 seconds]
The Perfect Capacitor

- A perfect capacitor combines linear and non-linear capacitance with remanent polarization.

This capacitor is not as square as the one for which the remanent polarization was plotted as the nCV three pages back. This capacitor has much smaller peaks which allow the structure at the base of the nCV to be seen in perspective.
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**C\textsubscript{FE} Equation**

The three components identified for this discussion are combined below to create a single equation for FE capacitance. (\(C_{\text{diode}}\) will be ignored.)

- **Towards \(V_{\text{Max}}\):**

\[
C_{\text{FE}} = C_{\text{Linear}} + \frac{C_{\text{Paraelectric}}}{\sigma_{\text{Paraelectric}} \sqrt{2\pi}} e^{-\left[\frac{V-V_{\text{Offset}}}{2\sigma_{\text{Paraelectric}}}\right]^2} + M \frac{C_{\text{Remanent}}}{\sigma_{\text{Remanent}} \sqrt{2\pi}} e^{-\left[\frac{(V-V_{\text{c}}^+)}{2\sigma_{\text{Remanent}}}\right]^2} + C_{\text{Diodes}}
\]

\(M = 1\) for switching or \(M = 0\) for non-switching

- **Return-to-Zero:**

\[
C_{\text{FE}} = C_{\text{Linear}} + \frac{C_{\text{Paraelectric}}}{\sigma_{\text{Paraelectric}} \sqrt{2\pi}} e^{-\left[\frac{V-V_{\text{Offset}}}{2\sigma_{\text{Paraelectric}}}\right]^2} - C_{\text{Diodes}}
\]
The derivative of a real loop (dotted) can be hand-fitted by the components.
Fitted Components

- Summation of the fitted components against the original loop.
An FE Cap in a Circuit

The equation describing the capacitance of a ferroelectric capacitor can now be inserted directly into the classic Resistor-Capacitor Charging equation from electrical engineering. This equation can be rigorously derived so the substitution is justified.

\[
V_{out} = V_{pwr} \cdot (1 - e^{-\frac{t}{RC_{FE}}})
\]

In the following pages, the impact of the ferroelectric capacitor properties on circuit performance is demonstrated.
Classic RC

A ferroelectric capacitor will exhibit multiple capacitances when switching. The charging of two different linear capacitors is below. They follow the classic equation:

\[ V_{out} = V_{pwr} \cdot (1 - e^{\frac{-t}{RC}}) \]

![Graph showing charging curves for different capacitances](image)
To model a simple ferroelectric capacitor $C_{FE}$, use a smaller capacitance when remanent polarization is *not switching* and a higher capacitance when it *is switching*, in this case from 2.2 volts to 2.9 volts.
A Real $RC_{FE}$

Measured

A real ferroelectric capacitor follows this model exactly with its non-linear capacitances defined by the $C_{FE}$ equation derived earlier.

$C = 400 \, \mu m^2 \ 2600\AA$-thick $20/80$ PZT = \textit{linear + non-linear + remanent polarization}

$R = 15M\Omega$

Defined as the “Shelf Voltage”.
The switching and non-switching curves below are the result of the limitation of current flow by the resistor and are not ‘intrinsic’ switching speed curves. The ferroelectric capacitor will explicitly follow the \( \text{RC}_{\text{FE}} \) rise time law as long as the intrinsic switching speed of the ferroelectric capacitor is faster than \( \text{RC}_{\text{FE}} \).
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KAI vs NLS vs RC\textsubscript{FE}

a) The Kolmogorov-Avrami-Ishibashi domain switching theory posits \textit{nucleation-dominated switching}.

\[ P = P_0 \left( 1 - e^{\frac{-t}{t_0}} \right) \]

b) The Nucleation-Limited Switching (NLS) model attempts to correct KAI when there are few nucleation sites.

\[ P = P_0 \left( 1 - \langle e^{\frac{-t}{t_i}} \rangle \right) \]

b) If the ferroelectric material is faster than the tester, the classic electrical engineering equation applies. (RC\textsubscript{FE})

\[ P = P_0 \left( 1 - e^{\frac{-t}{RC_{FE}}} \right) \]

KAI vs NLS vs $RC_{FE}$

This classic paper shows a Shelf Voltage!

FIG. 4. Fitting of the time dependence of the switched area for the 1.2 V bias by the KAI function $q(t) = 1 - \exp\left(-\left(t/t_0\right)^n\right)$ (solid line) and by the NLS model (see Ref. 27) (dashed line).

KAI vs NLS vs $RC_{FE}$

a) The presence of the shelf voltage in the Gruverman et al data means that this test was resistance limited and followed the $RC_{FE}$ rule as a circuit component.

b) The test circuit resistance slows down the capacitor response but the ferroelectric switching mechanism(s) define the capacitance versus voltage response of the capacitor.

\[
P = P_0 \left(1 - e^{\frac{-t}{RC_{FE}}}\right)
\]

Conclusion: the shape of the ferroelectric switching function (KAI, NLS, etc) is retained in all such measurements no matter how slow. The intrinsic switching time constant is not.
Correction to KAI & NLS

a) Note the asymmetry of the three equations. KAI and NLS have only a circuit-independent time constant in the denominator of the power of the exponential.

\[ P = P_0 \left( 1 - e^{\frac{-t^2}{t_0}} \right) \]
\[ P = P_0 \left( 1 - \langle e^{\frac{-t}{t_i}} \rangle \right) \]
\[ P = P_0 \left( 1 - e^{\frac{-t}{RC_{FE}}} \right) \]

b) The RC_{FE} Law equation ignores switching physics.
Correction to KAI & NLS

Both the circuit law and the switching physics operate simultaneously. The slower mechanism dominates so the two mechanisms should be treated as components in series.

The time constant should be ‘$RC_{FE} + t_{\text{characteristic}}$’.

This correction is recursive since the value of $C_{FE}$ depends on $t_c$. Simulations may not converge if $RC_{FE}$ and $t_c$ are nearly equal in magnitude.

\[
P = P_0 \left( 1 - e^{\frac{-t}{RC_{FE} + t_0}} \right)^2
\]

\[
P = P_0 \left( 1 - e^{\frac{-t}{RC_{FE} + t_i}} \right)
\]

\[
P = P_0 \left( 1 - e^{\frac{-t}{RC_{FE} + t_c}} \right)
\]
Cold Nucleation

All switching theories treat domain reversal as an activation energy mediated process.

\[ t_{nucleate} = t_{attempt} \left( e^{\frac{E_{Activation}}{kT}} \right) \]

Rappe et al. predict from first principles that the nucleation activation energy for Lead Titanate should increase by a factor of \( \sim 4 \) while decreasing the temperature from ambient to 200K. This should slow down the rate of reverse domain nucleation by a factor of \( e^4 \).

*This does not happen in thin film PZT at normal test speeds!*

Cold Nucleation

Hysteresis @ 20V 10k->310K
[ AB403 20/80 PZT 2600A ]
Cold Nucleation

- Switched Remanent Polarization vs Frequency from a temperature of 250 K down to 50 K shows no change whatsoever in switching speed with temperature.
Analysis

• The temperature independence of the remanent polarization switching speed may be an indication that it is a function of tunneling, not nucleation rates.

• The nucleation rate model is preserved if the nucleation time constant is so fast compared to the maximum test frequency that even an $e^4$ slow-down in nucleation rate would still cause domain switching to be faster than the $RC_{FE}$ circuit speed limitation.

• Preserving the nucleation rate models given the megahertz speed of the cryogenic PUND tests would thus require PZT switching to occur with a 10 picosecond time constant at room temperature.
What Determines Vc?

- Why does the Coercive Voltage change with voltage for BFO and PZT?

How can the coercive voltage for remanent polarization switching be predicted from existing models?
Leakage Measurement

The polarization at the top of a pulse applied to a PZT capacitor continues to climb after the pulse voltage is stable.

This climb is usually associated with current leakage through the capacitor at voltage.
Vortices or Leakage?

The Leakage Measurement simply measures the change in charge coming from the capacitor after the applied voltage has stabilized across the capacitor.

\[
I = \frac{\Sigma Q}{\Delta t}
\]

Might vortex pair annihilation be hidden in this current?
Partial Switching

The voltage applied to the capacitor can stop anywhere along the Shelf Voltage and the capacitor will stay in that partially switched state. It has memory. *Polarization models need to explain this property.*
Conclusion

• Everything that happens inside a capacitor must appear in a measurement when the capacitor is hooked to a tester.

• Only two limitations will prevent the tester from observing an event:
  1. Does some charge event occur in parallel with an equal but opposite charge event that cancel each other?
  2. Is the signal too small?

• There remain many mysteries about ferroelectric capacitors.