

Fig 1: Ferroelectric capacitor element

Form: capacitorferroelectric:<instance name> n1 n2 <parameter list> n1, n2 are the element terminals

Parameters:

| Parameter | Type | Default Value | Required? |
|---|--------|---------------|-----------|
| epsid: Interfacial capacitance | DOUBLE | 32e-3 | no |
| density (F/m ²) | | | |
| epsb0: Bulk capacitance zero-bias | DOUBLE | 170 | no |
| permittivity (F/m) | | | |
| a: Area of cross-section of the | DOUBLE | n/a | yes |
| parallel plate capacitor (m ²⁾ | | | |
| d: Total capacitor thickness (m) | DOUBLE | n/a | yes |
| t: 2 * (Interfacial Capacitor | DOUBLE | 5e-9 | no |
| thickness at the plate dielectric | | | |
| interface) (m) | | | |
| k: Fringing capacitance constant (F) | DOUBLE | 1.6e-15 | no |
| alpha3: Describes the non-linearity | DOUBLE | 3.3e-3 | no |
| of the material in the Landau- | | | |
| Devonshire-Ginzburg model | | | |
| (m^2/C^2F) | | | |
| T0: Curie-Weiss temperature for a | DOUBLE | -167 | no |
| particular BST film thickness (deg | | | |
| C) | | | |
| T: Current Temperature of the | DOUBLE | -73 | no |
| sample (deg C) | | | |
| beta: Temperature Coefficient of | DOUBLE | 600 | no |
| Capacitance (TCC) at zero bias | | | |
| (ppm/deg C) | | | |
| p: Device periphery for fringing | DOUBLE | n/a | yes |
| capacitance calculations (m) | | | |

Example:

.model c_ferro capacitorferroelectric (epsid =50e-3 epsb0=170 a=2000e-12 t=5e-9 + k=2.0e-15 alpha3=3.3e-3 T0=-167 T=-80 beta=1000 p=240e-9) capacitorferroelectric: cf1 3 0 model="c_ferro" d=125e-9

Details:

This element models a non-linear ferroelectric capacitor. A parallel plate physical model of the capacitor is considered although this concept can be further extended to model ferroelectric IDCs (inter-digitated capacitors) and gap capacitors. This model accounts for interfacial, bulk capacitance and fringing capacitance. It also considers thickness and temperature dependence of the high-permittivity ferroelectric material. This model can be used during time-domain analysis. Leakage and breakdown currents are not modeled.

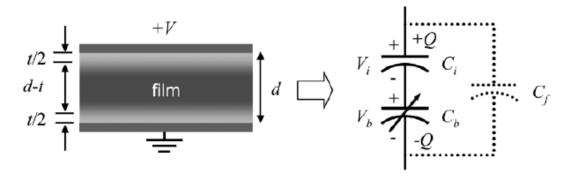


Fig 2: Ferroelectric capacitor model that includes the effect of the interfacial capacitance, bulk capacitance and fringing capacitance[2].

Data collected from experiments indicates that a "dead" layer non-tunable capacitance exists in series with a bulk non-linear capacitance. The voltage applied is dropped across a series combination of the interface capacitance at the two plate dielectric interfaces and the bulk ferroelectric dielectric material. While this model characterizes large area capacitors ($\approx 2000um^2$) very well, small area capacitors need an additional fringing capacitance in parallel as shown in Fig. 2 to account for their reduced tunability compared to large area capacitors[2]. This model ignores the space-charge buildup near the electrodes.

With reference to Fig 2, both the interfacial capacitances are collectively described by a linear charge-voltage equation:

$$V_{i} \frac{Q}{Ci}; Ci = \frac{\varepsilon_i A}{t}$$
 (1.1)

Here the interfacial capacitance density $\frac{\mathcal{E}_i}{t}$ is determined experimentally from a series of devices of varying thickness.

The bulk is described by a nonlinear equation from the Landau-Devonshire-Ginzburg (LDG) model [1] by:

$$V_b = \frac{Q}{C_{b,\text{max}}} + KQ^3 \tag{1.2}$$

$$\frac{1}{C_{h \max}} = \alpha_1 \frac{(d-t)}{A} \text{ and } K = \alpha_3 \frac{(d-t)}{A}$$
 (1.3)

The total voltage across the device is then:

$$Vcap = Q(\frac{1}{C_i} + \frac{1}{C_{b,\text{max}}}) + KQ^3$$
 (1.4)

The fringing capacitance is independent of the field and thickness and is given by

$$C_f = k \frac{P}{d} \tag{1.5}$$

$$\varepsilon_{b}(T) \approx \varepsilon_{b0} [1 - \beta (T - T0)] \tag{1.6}$$

In the equations above

 ε_i = Interfacial material dielectric permittivity (F/m²)

 ε_{b0} = Bulk dielectric material zero-bias permittivity (F/m)

A =Area of cross-section of the parallel plate capacitor (m²)

d = Total capacitor thickness (m)

t = Interfacial capacitance thickness (m)

k = Fringing capacitance constant (F)

 α_3 = Describes the non-linearity of the material in the Landau-Devonshire-Ginzburg model (m²/C²F)

 $\varepsilon_h(T)$ = Temperature dependent bulk dielectric zero-bias permittivity (F/m)

 β = Temperature Coefficient of capacitance (TCC) at zero bias (ppm/deg C)

T =Current Temperature of the sample (deg C)

 T_0 = Curie-Weiss temperature for a particular BST film thickness (deg C)

Q =Charge on the capacitor (C)

Netlist file circuit:

The netlist model used to prove the correctness of the model is a RC coupling circuit. The netlist is run with three different values of output resistance 'R' to change the RC time-constant of the circuit as shown in the fig 3. The input square wave changes shape based on the RC time constant in comparison with the 'T' – the time period of the square wave.

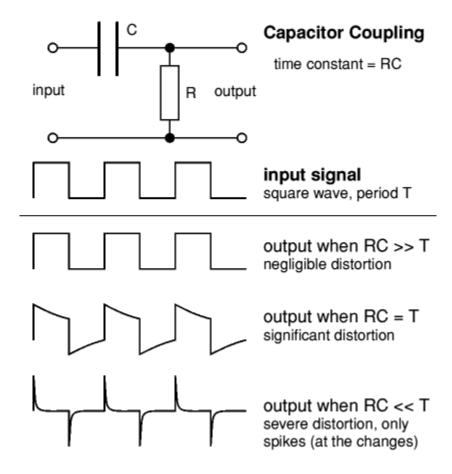


Fig3. Input square wave and output signal wave shapes based on the RC time constant value in comparison with 'T' – the time period of the wave [6].

Example of Transient analysis (.TRAN2) Fixed time steps, time-stepping nonlinear analysis

Netlist File:

*** Transient Analysis for the Ferroelectric capacitor

.options verbose

```
*.svtr tstop = 2e-5 \text{ n\_freqs} = 70 \text{ tstep} = 0.25e-6
*.svtr tstop = 1e-4 \text{ n\_freqs} = 70 \text{ tstep} = 0.25e-6
.tran2 tstop = 1e-4 tstep = 0.50e-6 out\_steps=1 im=2
*vsource:1 1 0 vac=1.0 f=0.3e5 phase=90
vpulse:v1 1 0 v1=0 v2=5 td=0 tr=0.05e-5 tf=0.05e-5 pw=1.5e-5 per=3.5e-5
capacitorferroelectric:cf1 1 2 a=6500e-12 d=150e-9 p=160e-9
*RC time constant << T
*resistor:rin1 2 0 r=1000
*RC time constant ~ T
*resistor:rin1 2 0 r=25000
*RC time constant >> T
resistor:rin1 2 0 r=1000000
.options gnuplot
*.options postamble1 = "using 2:3"
.options plotVT1Preamble="set term x11 font 'helvetica,13';
set title 'Ferroelectric capacitor Voltage';
set xlabel 'TIME (microseconds)'; set ylabel 'VOLTAGE (V)'"
.out plot element "capacitorferroelectric:cf1" 0 ut 1e6 scalex plotVT1Preamble in
"capacitorferroelectric_v.out"
.options plotVT1Preamble="set term x11 font 'helvetica,13';
set title 'Ferroelectric capacitor Current';
set xlabel 'TIME (microseconds)'; set ylabel 'Current (A)'"
out plot element "capacitorferroelectric:cf1" 0 it 1e6 scalex plotVT1Preamble in
"capacitorferroelectric i.out"
.options plotVT1Preamble="set term x11 font 'helvetica,13';
set title 'Input Voltage Source';
set xlabel 'TIME (microseconds)'; set ylabel 'Voltage (V)'"
.out plot term 1 vt 1e6 scalex plotVT1Preamble in "source_v.out"
.options plotVT1Preamble="set term x11 font 'helvetica,13';
set title 'Voltage across resistor';
set xlabel 'TIME (microseconds)'; set ylabel 'Voltage (V)'"
.out plot term 2 vt 1e6 scalex plotVT1Preamble in "res v.out"
*pack in "capacitorferroelectric_combo.out"
```

```
*.out plot "capacitorferroelectric_combo.out" postamble
```

.end

```
Log File:
****** fREEDA 1.3 running on Sun Apr 20 22:54:49 2008 *******
 *** Parsing input netlist ...
 *** Expanding subcircuits ... done.
 *** Initializing Elements ...cmax: 2.08002e-10
done.
 *** Checking reference terminals ... done.
 *** Starting analysis ...
 Matrix size = 3
 Matrix nnz = 6
 equed = 7.95719e-305
 recip_pivot_growth = 1
 1 / Condition number = 0.840131
 info = 0
 ferr = 9.70941e-308
 berr = 1
 No of nonzeros in factor L = 6
 No of nonzeros in factor U = 6
 No of nonzeros in L+U=9
                     total MB needed 0.001
 L\U MB 0.000
                                                  expansions 0
 Using line search method.
 Nonlinear analysis tolerance (ftol) = 6.12865e-06
 Maximum number of nonlinear iterations per time-point (maxit) = 250
 Using Lee and Lee's quasi-Newton updates.
 --- Starting transient simulation ...
```

Number of nonlinear state variables: 1

| Step | Time (s) | Residual | Recent Max | | Max | |
|------|----------|----------|---|--|-----|---|
| | | ' | e+00 0.000000e+00 -13 6.274981e-13 | | | ' |

^{**.}out plot element "capacitorferroelectric22:cf1" 0 xt in "capacitorferroelectric_x.out"

^{*.}out plot element "capacitorferroelectric22:cf1" 0 ut stripx in

[&]quot;capacitorferroelectric_v.out"

```
2 | 1.000000e-06 | 1.785239e-13 | 1.785239e-13
                                                      | 6.274981e-13 |
    3 | 1.500000e-06 | 1.865175e-14 | 1.865175e-14
                                                     6.274981e-13
    4 | 2.000000e-06 | 1.152591e-01 | 1.152591e-01 | *| 1.152591e-01 |
    5 | 2.500000e-06 | 1.152591e-01 | 1.152591e-01
                                                     * | 1.152591e-01 |
    6 | 3.000000e-06 | 1.152591e-01 | 1.152591e-01
                                                     * | 1.152591e-01 |
    7 | 3.500000e-06 | 1.152591e-01 | 1.152591e-01
                                                    * | 1.152591e-01 |
    8 | 4.000000e-06 | 1.152591e-01 | 1.152591e-01
                                                     * | 1.152591e-01 |
    9 | 4.500000e-06 | 1.152591e-01 | 1.152591e-01
                                                     * | 1.152591e-01 |
   10 | 5.000000e-06 | 1.152591e-01 | 1.152591e-01
                                                     * | 1.152591e-01 |
:
                                                                     :
   190 | 9.500000e-05 | 1.124087e-01 | 1.124087e-01 *| 1.152591e-01 |
   191 | 9.550000e-05 | 1.124087e-01 | 1.124087e-01 * | 1.152591e-01 |
   192 | 9.600000e-05 | 1.124087e-01 | 1.124087e-01 * | 1.152591e-01 |
   193 | 9.650000e-05 | 1.124087e-01 | 1.124087e-01 *| 1.152591e-01 |
   194 | 9.700000e-05 | 1.124087e-01 | 1.124087e-01 * | 1.152591e-01 |
   195 | 9.750000e-05 | 1.124087e-01 | 1.124087e-01 *| 1.152591e-01 |
   196 | 9.800000e-05 | 1.124087e-01 | 1.124087e-01 * | 1.152591e-01 |
   197 | 9.850000e-05 | 1.124087e-01 | 1.124087e-01 *| 1.152591e-01 |
   198 | 9.900000e-05 | 1.124087e-01 | 1.124087e-01 * | 1.152591e-01 |
   199 | 9.950000e-05 | 1.124087e-01 | 1.124087e-01 * | 1.152591e-01 |
  200 | 1.000000e-04 | 1.124087e-01 | 1.124087e-01 * | 1.152591e-01 |
--- Maximum Residual: 0.115259
```

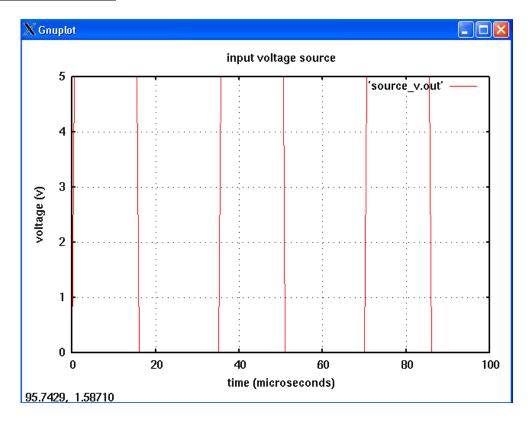
Plotting output file: capacitorferroelectric_v.out. Plotting output file: capacitorferroelectric_i.out.

Plotting output file: source_v.out. Plotting output file: res_v.out.

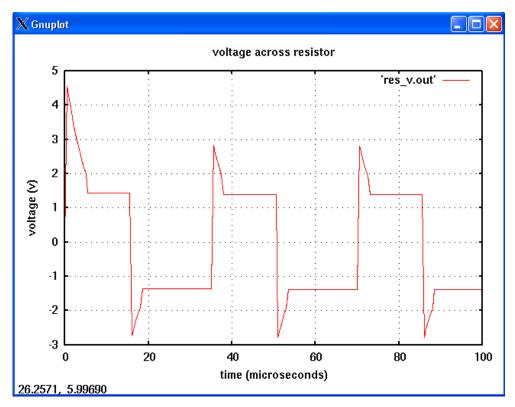
****** fREEDA 1.3 stopping on Sun Apr 20 22:54:52 2008 ********

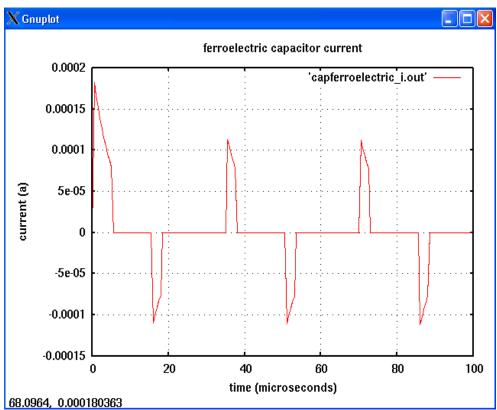
Simulation Results in fREEDA:

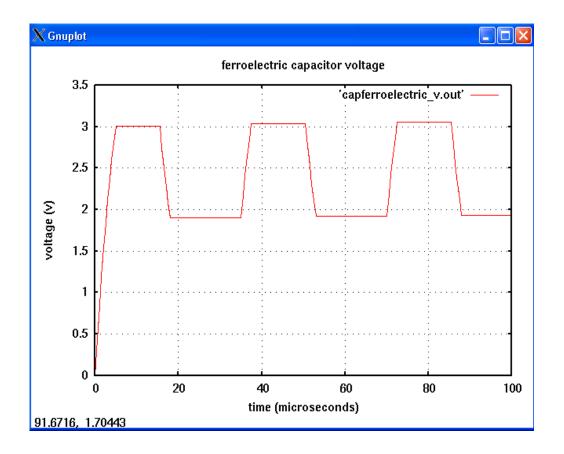
Input Voltage Pulse:



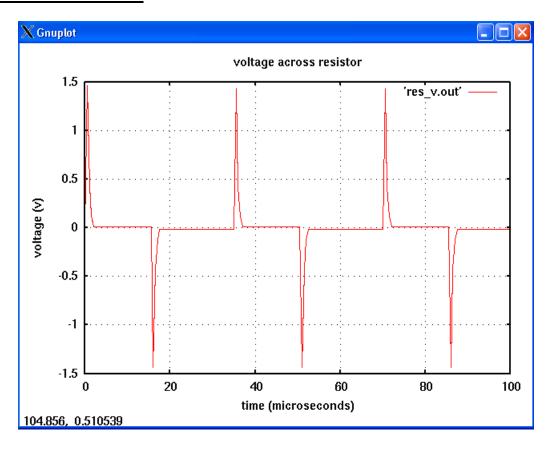
RC time constant ~ T:

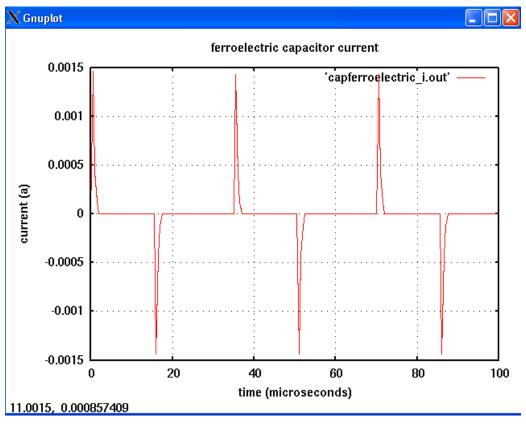


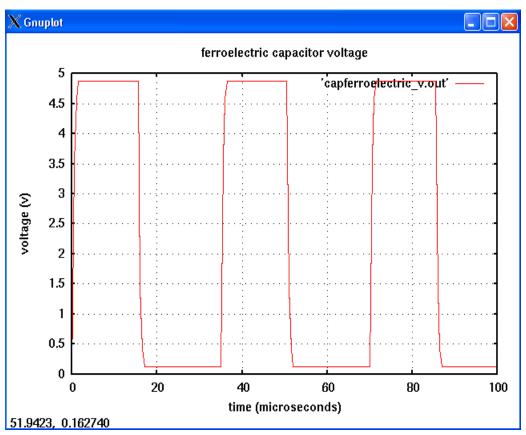




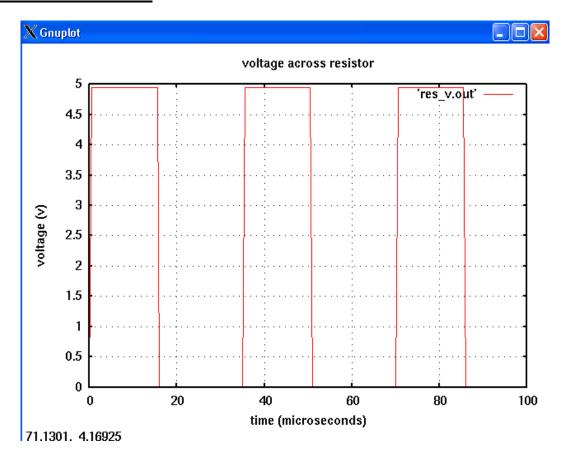
RC time constant << T:

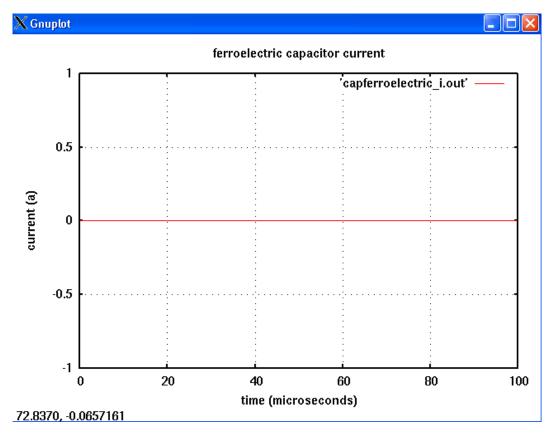


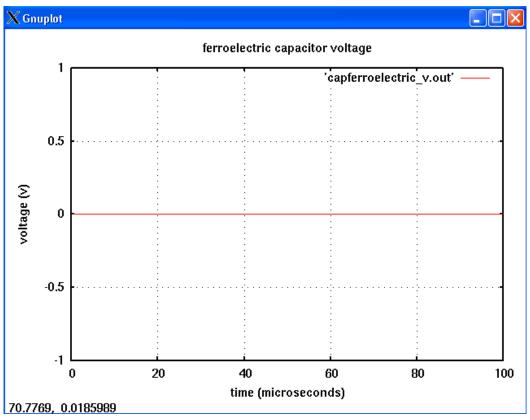




RC time constant >> T:







Version:

2008.04.20(2008 April 20)

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|----------------|---|
| | |

| Name | Affiliation | Date | Links nc state university |
|-----------------------------------|---------------------|------------|---------------------------|
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References:

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- [2] Michael B. Steer, W. Devereux Palmer, Robert York, "Multifunctional Adaptive Microwave Circuits and systems", Chap 4, 2008 Edition
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- [6] http://www.kpsec.freeuk.com/capacit.htm