Verilog-A model for ferroelectrics in organic electronics

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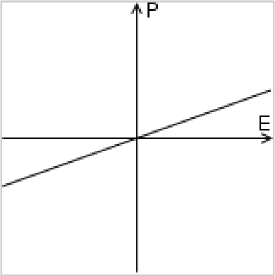
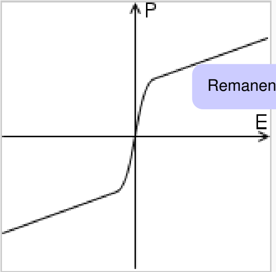
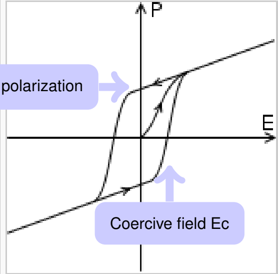
Ferroelectricity



Dielectric polarization



Paraelectric polarization



Remanent polarization

Coercive field Ec

Ferroelectric polarization

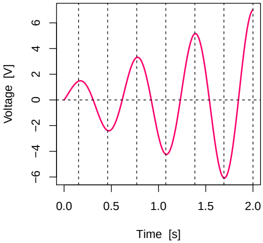
- Electric displacement: $\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} = \varepsilon_0 (1 + \chi) \mathbf{E} = \varepsilon_0 \varepsilon_r \mathbf{E}$
- `http://en.wikipedia.org/wiki/Ferroelectricity`

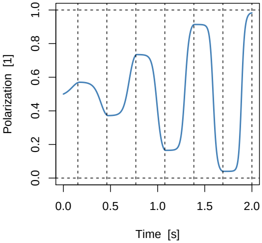
Ferroelectric model equations

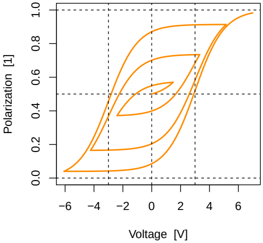
up sweep, $V_\mathrm{i} < V_\mathrm{f}$	down sweep, $V_\mathrm{f} < V_\mathrm{i}$
$\frac{\mathrm{d}p_\uparrow}{\mathrm{d}V} = (1 - p_\uparrow) f_\uparrow$	$\frac{\mathrm{d}p_\uparrow}{\mathrm{d}V} = p_\uparrow f_\downarrow$
$f_\uparrow(V) = \frac{1}{V_0} \frac{1}{1 + \exp[(V_\mathrm{c} - V)/V_0]}$	$f_\downarrow(V) = \frac{1}{V_0} \frac{1}{1 + \exp[(V_\mathrm{c} + V)/V_0]}$
$p_{\uparrow\mathrm{f}} = 1 - (1 - p_{\uparrow\mathrm{i}}) \frac{1 + \exp[(V_\mathrm{i} - V_\mathrm{c})/V_0]}{1 + \exp[(V_\mathrm{f} - V_\mathrm{c})/V_0]}$	$p_{\uparrow\mathrm{f}} = p_{\uparrow\mathrm{i}} \frac{1 + \exp[(-V_\mathrm{i} - V_\mathrm{c})/V_0]}{1 + \exp[(-V_\mathrm{f} - V_\mathrm{c})/V_0]}$
$C = 2\,P_\mathrm{s}\,(1 - p_\uparrow)\,f_\uparrow = 2\,P_\mathrm{s}\,\mathrm{d}p_\uparrow/\mathrm{d}V$	$C = 2\,P_\mathrm{s}\,p_\uparrow\,f_\downarrow = 2\,P_\mathrm{s}\,\mathrm{d}p_\uparrow/\mathrm{d}V$

- Polarization $p_\uparrow \in [0:1]$, neutral value $p_\uparrow = 0.5$
- Three model parameters V_c, P_s, V_0
- S J Hong *et al.*, 2002

Ferroelectric hysteresis







- Counter-clockwise hysteresis loop
- Coercive voltage: $V_c = 3.0\,\text{V}$
- Thermal voltage: $V_0 = 1.0\,\text{V}$

A first implementation via Verilog-A

```
v = V(px);
I(drv) <+ ddt(v);
I(drv) <+ -V(drv);
u = V(drv);
@ (initial_instance)
begin
  v_ini = 0.0;
  p_ini = 0.5;
  v_prv = v;
end
// Polarization [1] for both up and down sweep
p_up = 1.0 - (1.0 - p_ini)*(1.0 + exp((v_ini - vc)/v0))/
        (1.0 + exp((v - vc)/v0));
p_dn = p_ini*(1.0 + exp((-v_ini - vc)/v0))/
        (1.0 + exp((-v - vc)/v0));
p = .5*(p_up + p_dn) + .5*(p_up - p_dn)*tanh((v - v_prv)/`eps);
// Ferroelectric capacitance [F/cm2] from polarization
c_up = 2.0*ps*(1.0 - p)/(1.0 + limexp((vc - v)/v0))/v0;
c_dn = 2.0*ps*p/(1.0 + limexp((vc + v)/v0))/v0;
c = .5*(c_up + c_dn) + .5*(c_up - c_dn)*tanh((v - v_prv)/`eps);
// Current contributions [A]
I(px) <+ dpix*dpix*c*u;
I(px) <+ dpix*dpix*v/cgr;
// Update voltage, polarization
v_ini = v;
p_ini = p;
// Store voltage for next step
v_prv = v;
```

Voltage derivative

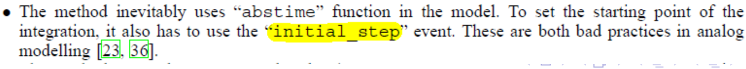
Initial condition

ODE solution

Capacitance from polarization

Current computation

Update initial condition



- The method inevitably uses "`abstime`" function in the model. To set the starting point of the integration, it also has to use the "`initial_step`" event. These are both bad practices in analog modelling [23, 36].

Another implementation of the same model

```
v = V(pix, top);
// Voltage time derivative [V/s]
I(drv, gnd) <+ ddt(v);
I(drv, gnd) <+ -V(drv, gnd);
u = V(drv, gnd);
// Voltage dependent driving direction [1]
w = tanh(u/‘eps);
I(dir, gnd) <+ w - V(dir, gnd);
// Voltage dependent polarization transition rate [1/V]
f_up = 1.0/(1.0 + limexp((vc - v)/v0))/v0;
f_dn = 1.0/(1.0 + limexp((vc + v)/v0))/v0;
// dp/dv [1/V] for both up and down sweep
p = V(pol, gnd);
dp_up = (1.0 - p)*f_up;
dp_dn = p*f_dn;
dpdv = .5*(dp_up + dp_dn) + .5*(dp_up - dp_dn)*w;
// Enforce ODE for polarization [1]
I(pol, gnd) <+ dpdv*u;
I(pol, gnd) <+ ddt(-p);
// Ferroelectric capacitance [F/cm2] from polarization
c_up = 2.0*ps*(1.0 - p)*f_up;
c_dn = 2.0*ps*p*f_dn;
if (w == 0)
  c = .5*(c_up + c_dn);
else
  c = .5*(c_up + c_dn) + .5*(c_up - c_dn)*w;
// Current contributions [A]
I(pix, top) <+ dpix*dpix*c*u;
I(pix, top) <+ dpix*dpix*v/cgr;
```

Voltage derivative

State variable: up/down

Rate of polarization change

Polarization increment

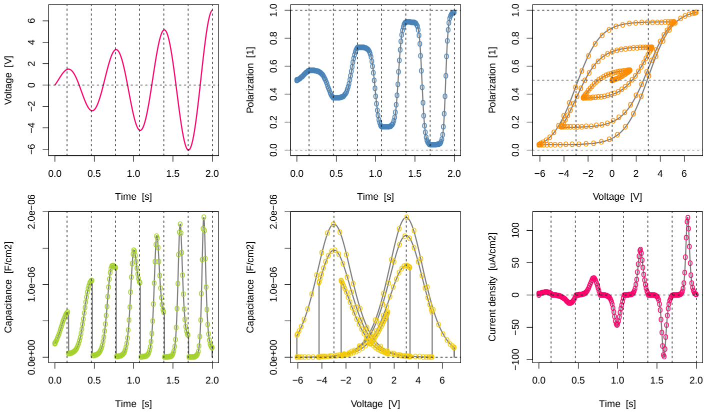
ODE left for solver

Capacitance from polarization

Current computation

- T Wang / J Roydchowdhury, 2016

CV simulation of a ferroelectric



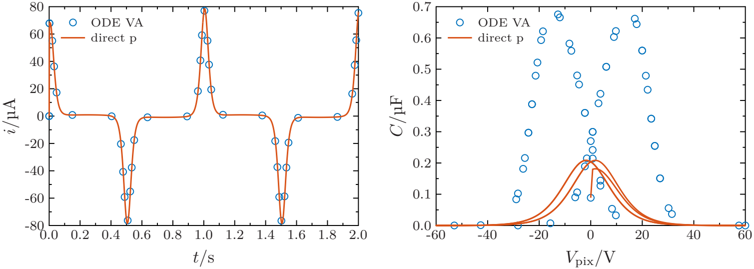
- Comparison of the two model implementations (color vs. gray)
- Hysteresis leads to double peak of the CV curve
- Discontinuous capacitance values

Comparison of both implementations

	1$^{\mathrm{st}}$ implementation	2$^{\mathrm{nd}}$ implementation
Character	ill–posed	well–posed
State variables	none	up/down, polarization
`.options timeint`	`maxord = 1`	`erroption = 1`
Max time step	`1m`	`10m`
Time steps	2026	206
Run time [real]	0.770 s	0.476 s
Analysis	`.tran`, `.ac`	`.tran`

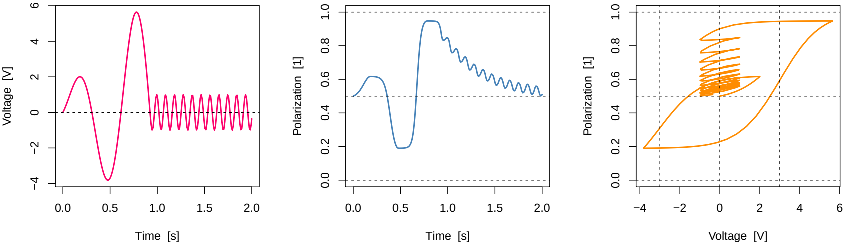
- All simulations using Xyce 6.6
- Compilation using ADMS 2.3.5 into shared object library
- Mainly `.tran` simulations only

.ac analysis does not work for ODE

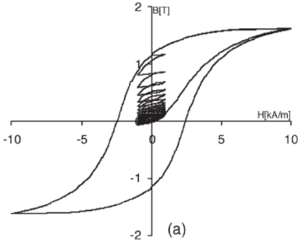


- ADMS inserts second derivatives into Jacobian matrix, because the first derivative is used in the VA code explicitly.
- This gives erroneous results in the second implementation.
- First implementation runs alright.

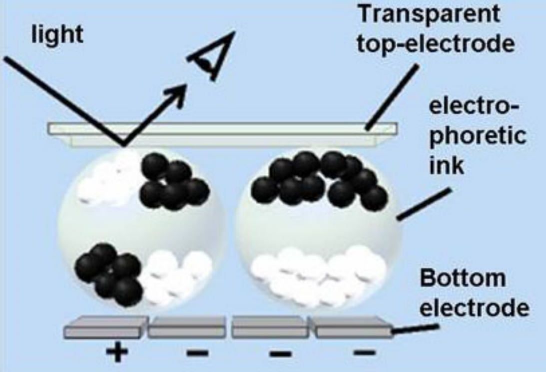
Minor hysteresis loop simulation



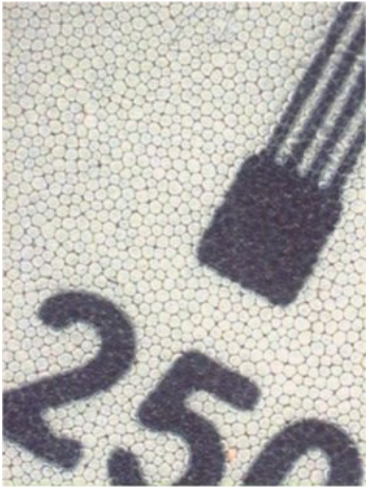
- During minor loops, the polarization relaxes towards equilibrium
- This simulation capability indicates robustness of the implementation
- Compare H Al–Junaid *et al.*, 2006



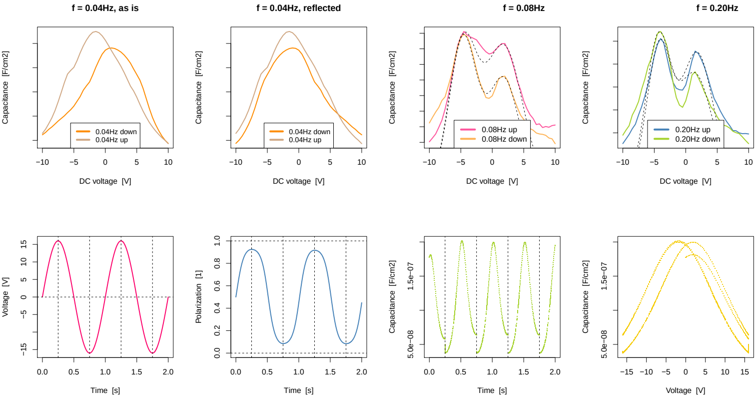
Electrophoretic medium




Flexible electrophoretic (E Ink)

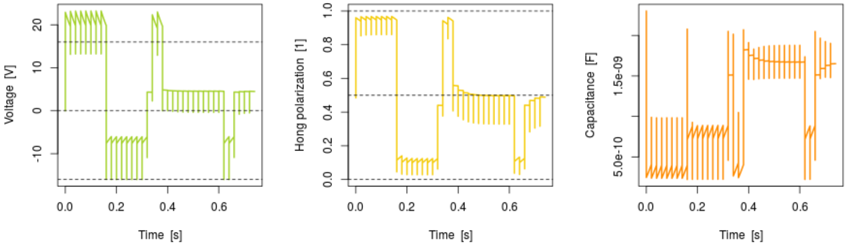


Parameter extraction via CV measurement

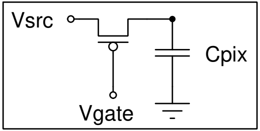


- CV curve follows double Gaussians
- Large thermal voltage dominates any constant capacitance
- Frequency independent peak position and width

Simulation of a pixel transition

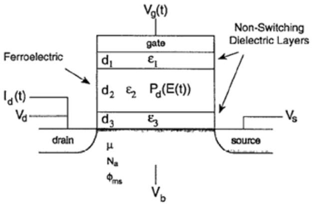


- Three possible source voltages: V_{srcpos}, V_{srcneg}, and null frame
- Final null frames to reach neutral polarization
- Capacitance changes by 4×
- Has to be linked up with optical measurements

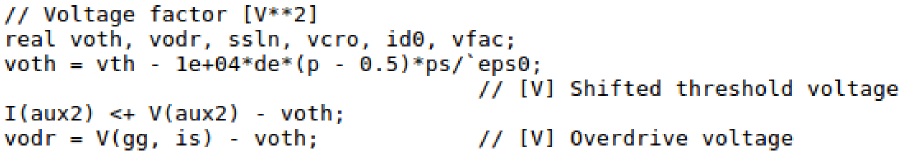


Ferroelectric threshold voltage shift

$$
\begin{aligned}
I = -\frac{W}{L}\,\frac{\mu\, C_{\mathrm{stack}}}{\beta^2}\Bigg[& \left(1+\beta\, V_{\mathrm{gb}}+\frac{\beta\, d_2}{\varepsilon_0\varepsilon_2}\,P_{\mathrm{d}}(E_2)\right)(\beta\,\Phi_{\mathrm{sL}}-\beta\,\Phi_{\mathrm{s0}}) \\
& -\frac{1}{2}\left[(\beta\,\Phi_{\mathrm{sL}})^2-(\beta\,\Phi_{\mathrm{s0}})^2\right]-\frac{2}{3}\,a\left[(\beta\,\Phi_{\mathrm{sL}})^{3/2}-(\beta\,\Phi_{\mathrm{s0}})^{3/2}\right] \\
& + a\left[(\beta\,\Phi_{\mathrm{sL}})^{1/2}-(\beta\,\Phi_{\mathrm{s0}})^{1/2}\right]\Bigg]
\end{aligned}
$$

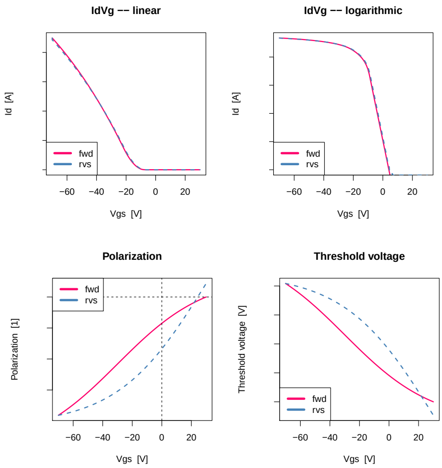


- $a = 0$, charge contribution of the depletion layer
- $\Phi_{\mathrm{sL}} - \Phi_{\mathrm{s0}} = V_{\mathrm{ds}}$ drain–source voltage
- S L Miller / P J McWorther, 1992
- A Saeidi *et al.*, 2016

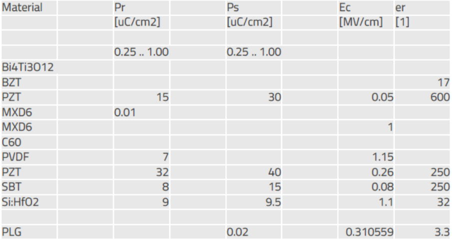


```
// Voltage factor [V**2]
real voth, vodr, ssln, vcro, id0, vfac;
voth = vth - 1e+04*de*(p - 0.5)*ps/`eps0;
                              // [V] Shifted threshold voltage
I(aux2) <+ V(aux2) - voth;
vodr = V(gg, is) - voth;      // [V] Overdrive voltage
```

IdVg including ferroelectrics



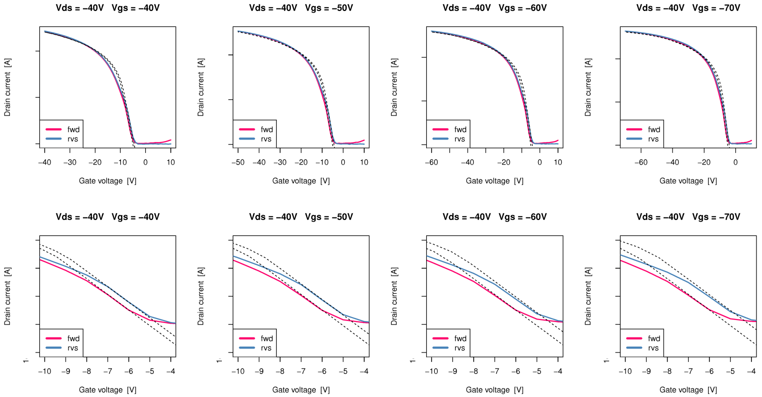
- Ferroelectric materials previously used with organic transistors, mainly for memory



Material		Pr		Ps		Ec	er
		[uC/cm2]		[uC/cm2]		[MV/cm]	[1]
		0.25 .. 1.00		0.25 .. 1.00			
Bi4Ti3O12							
BZT							17
PZT		15		30		0.05	600
MXD6		0.01					
MXD6						1	
C60							
PVDF		7				1.15	
PZT		32		40		0.26	250
SBT		8		15		0.08	250
Si:HfO2		9		9.5		1.1	32
PLG				0.02		0.310559	3.3

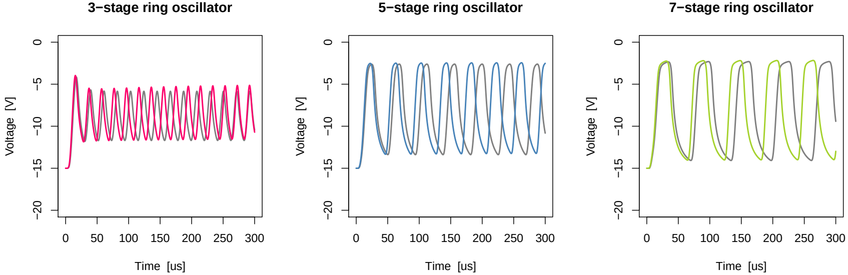
- After forward and reverse IdVg sweep, polarization is back to neutral level, approximately.

IdVg measurement and simulation

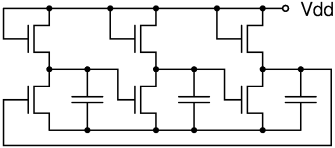


- Color: measurement, dashed: simulation
- Increase of $V_{\mathrm{th}}(\mathrm{rvs}) - V_{\mathrm{th}}(\mathrm{fwd})$ with increasing V_{gs} return value is predicted well by the ferroelectric model

Unipolar ferroelectric ring oscillator



3 stage ring oscillator



Narrow load transistor

Wide drive transistor

Small load capacitor

- frequency increase ≈ 10%

Summary / Outlook

- Due to the wide arsenal of materials in organic electronics, ferroelectrics are quite common
- Like ferromagnetics, ferroelectrics are interesting materials from a modeling point of view
- With increasing demands on the modeling accuracy, models of ferroelectrics will move into focus
- Two application examples were presented. Obviously, there are more: memory, ...