Wurtzite-Perovskite-Wurtzite (ZnO-BaTiO$_3$-ZnO) Interface Polarization Hysteresis Model

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Multifunctional 3D Heterostructures

D. E. Scharett and R. E. Garrison Arm. Log. **37** (2005).

Multi fuctional capabilities of **Future electronics**.

New concepts incorporate ferroelectric and piezoelectric properties into semiconductors to make multifunctional architectures for future device technology.

Here we introduce a multilayered structure prepared with wurtzite ZnO and perovskite BaTiO$_3$.

The coupling between the ZnO polarization (surface ionic polarization charge P_{sz}) and the switchable ferroelectric perovskite BaTiO$_3$ polarization P_d influences:

(I) Ferroelectric refractive index change Δn [1].
(II) Ferroelectric phase transition [2, 3].
(III) Electrical properties [4-6].
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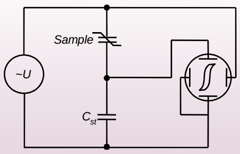
Experiment

ZnO, BaTiO$_3$ heterostructures are prepared by Pulsed Laser Deposition and subsequent masking with ohmic Pt back and front contacts.

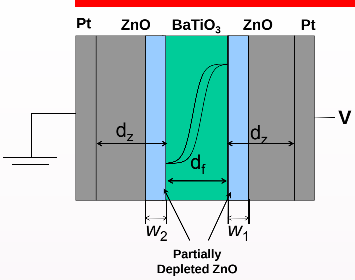
Electric Sawyer-Tower [5] measurements were performed on samples at 1.5 kHz frequency respectively.



Sawyer-Tower circuit

Electric Interface Polarization Coupling and Depletion Layer Model

Internal mechanism



Voltage destribution accross the structure:

$$V = d_f E_f + \frac{eN_c}{2\varepsilon_z}(w_1^2 - w_2^2).$$

Internal change mechanism:

$$V = \frac{d_f}{\varepsilon_f}\sigma_b - \frac{d_f}{\varepsilon_f}P_d - \frac{eN_c}{2\varepsilon_z}(w_2^2 - w1^2) - \frac{d_z}{\varepsilon_z}(P_{sz1} + P_{sz2}).$$

Boundary conditions at right and left ZnO-BaTiO$_3$interfaces:

$$eN_c w_1 + P_{sz1} = E_f\varepsilon_f + P_d,$$
$$-eN_c w_2 + P_{sz2} = E_f\varepsilon_f + P_d.$$

Different model cases and the dipole polarization

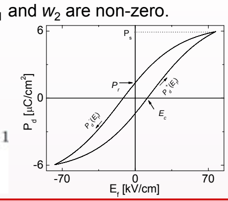
Depending on the applied bias four different model cases are possible:

Case I	:	Both depletion widths, w_1 and w_2 are zero.
Case II	:	Depletion width w_1 is zero but not w_2.
Case III	:	Depletion width w_2 is zero but not w_1.
CaseIV	:	Both depletion widths w_1 and w_2 are non-zero.

Dipole polariazion (P_d):

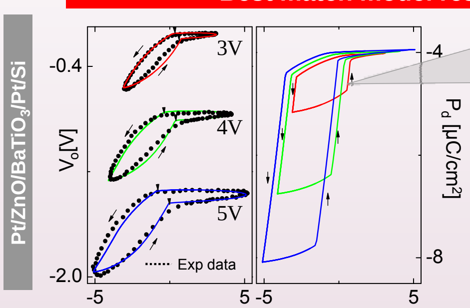
$$P_d^+(E_f) = P_s \tanh\left[\frac{(E_f - E_c)}{2\delta}\right]$$
$$P_d^-(E_f) = -P_d^+(-E_f)$$

where $\delta = E_c\left[\log\left(\frac{1+P_r/P_s}{1-P_r/P_s}\right)\right]^{-1}$

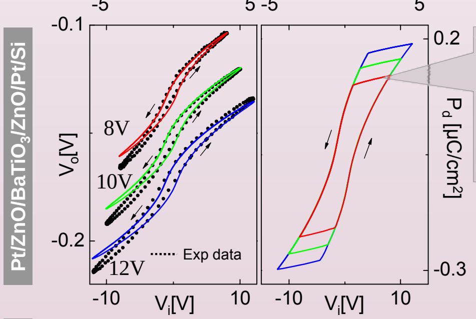


Experimental and Model Calculated Data

Best match model results



The ferroelectric properties of BaTiO$_3$ are influenced by the spontaneous polarization of ZnO (P_{sz}) and the depletion width of ZnO (w).

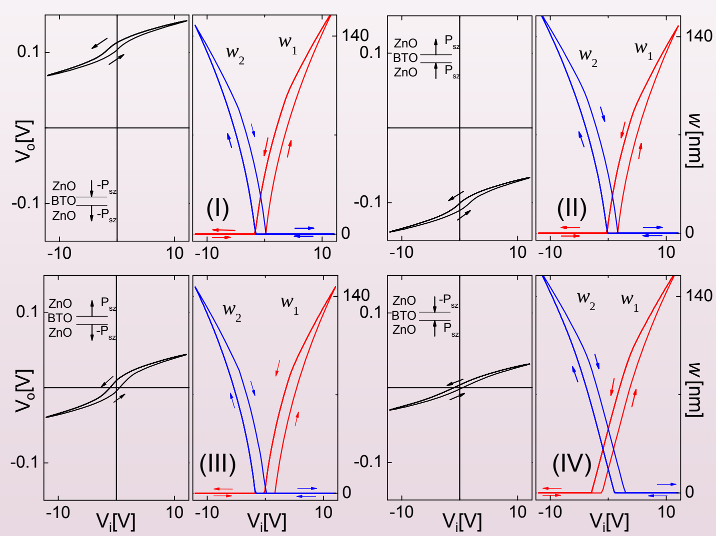


The ferroelectric properties of BaTiO$_3$ are influenced by the spontaneous polarization of both ZnO layers (P_{sz1}, P_{sz2}) and the depletion layers of top and bottom ZnO (w_1, w_2).

Model parameters

		ZnO/BaTiO$_3$	ZnO/BaTiO$_3$/ZnO
Coercive field (E_c)	V/m	1.1	1
Spontaneous polarization of BaTiO$_3$ (P_s)	µC/cm^2	14.1	2
Remanent polarization of BaTiO$_3$ (P_r)	µC/cm^2	5.64	0.06
Spontaneous polarization of ZnO (P_{sz})	µC/cm^2	-4.1	0.1
Overall sample resistance (R_s)	kΩ	13	420
Dielectric constant of BaTiO$_3$ (ε_f)		250	60
Dielectric constant of ZnO (ε_{zno})		8	8

Effect of ZnO polarity orientation in ZnO-BaTiO$_3$- ZnO



➢Orientation of spontaneous polarization of the ZnO layers controls the ferroelectric properties of the ZnO-BTO-ZnO structure.
➢Either positive or negative orientations of both spontaneous polariazions of ZnO layers results an asymmetry in the transport properties (different depletion layer endings in fig. (I) and (II)).
➢Asymmetric transport properties of the structure results in an asymmetric shift in the Sawyer-Tower response (shown in fig(I) and (II)).

[1] V. Voora *et al.*, *phys. stat. sol. (c)* **5**, 1328 (2008).
[2] M. Schubert *et al.*, *Ann. Phys.* **13**, 61 (2004).
[3] B. Mbenkum *et al.*, Appl. Phys. Lett. **86**, 091904 (2005).
[4] V. Voora *et al.*, J. Electron. Mater, **37**, 1029 (2008).
[5] N. Ashkenov *et al.*, Thin Solid Films **486**, 153 (2005).
[6] V. Voora *et al.*, Appl. Phys. Lett. **94**, 142904 (2009).

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