Wurtzite-Perovskite (ZnO-$BaTiO_3$) interface polarization hysteresis model

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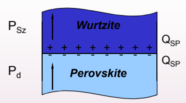
Polarization coupled interfaces

Wurtzite polarization (surface ionic charge) with the switchable ferroelectric perovskite polarization. This coupling influence:



(I) Ferroelectric refractive index change Δn
[*phys. stat. sol. (c)* **5**, 1328 (2008)].

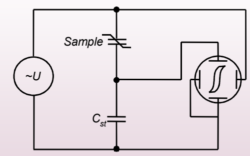
(II) Ferroelectric phase transition
[Ann. Phys. **13**, 61 (2004), Appl. Phys. Lett. **86**, 091904 (2005)].

(III) Electrical properties of junctions
[J. Electron. Mater, **37**, 1029 (2008), Thin Solid Films **486**, 153 (2005)].

Here we report:
Electrical and electrooptic measurements of $BaTiO_3$/ZnO structures.
- Generalized model to describe the Sawyer-Tower polarization hysteresis loops of our ZnO/BTO structures. The best fit model parameters are listed below.
- Index of refraction and piezoelectric thickness hysteresis behavior of our ZnO/BTO structures.

Experiment

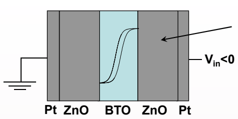
- Samples are prepared by Pulsed Laser Deposition and subsequent masking with ohmic Pt back and front contacts.
- Electric Sawyer-Tower and electrooptic ellipsometry measurements were performed on contacts and near contacts, respectively.



Sawyer-Tower circuit

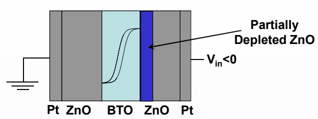
Generalized model for Sawyer-Tower response of ZnO-$BaTiO_3$ structures

Case I



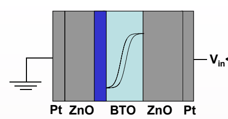
$$V = E_f d_f.$$
$$V = \sigma_b \frac{d_f}{\varepsilon_f} - P_d \frac{d_f}{\varepsilon_f}.$$

Case II



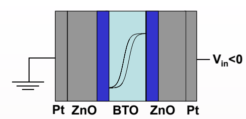
$$V = d_f E_f + \frac{eN_c w_1^2}{2\varepsilon_z}.$$
$$V = \frac{d_f}{\varepsilon_f}\sigma_b - \frac{d_f}{\varepsilon_f}P_d - \frac{d_z}{\varepsilon_z}P_{sz_1} + \frac{eN_c}{2\varepsilon_z}w_1^2.$$
$$eN_c w_1 + P_{sz_1} = E_f\varepsilon_f + P_d.$$

Case III



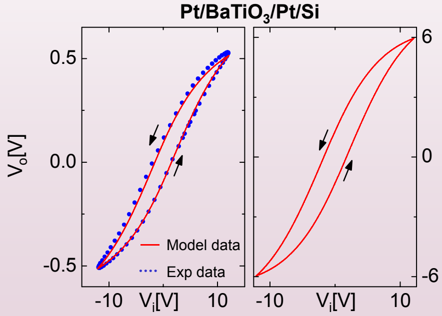
$$V = d_f E_f - \frac{eN_c w_2^2}{2\varepsilon_z}.$$
$$V = \frac{d_f}{\varepsilon_f}\sigma_b - \frac{d_f}{\varepsilon_f}P_d - \frac{d_z}{\varepsilon_z}P_{sz_2} - \frac{eN_c}{2\varepsilon_z}w_2^2.$$
$$-eN_c w_2 + P_{sz_2} = E_f\varepsilon_f + P_d.$$

Case IV

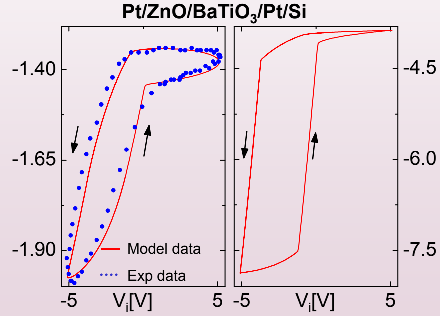


$$V = d_f E_f + \frac{eN_c}{2\varepsilon_z}(w_1^2 - w_2^2).$$
$$V = \frac{d_f}{\varepsilon_f}\sigma_b - \frac{d_f}{\varepsilon_f}P_d - \frac{eN_c}{2\varepsilon_z}(w_2^2 - w_1^2) - \frac{d_z}{\varepsilon_z}(P_{sz_1} + P_{sz_2}).$$
$$eN_c w_1 + P_{sz_1} = E_f\varepsilon_f + P_d.$$
$$-eN_c w_2 + P_{sz_2} = E_f\varepsilon_f + P_d.$$

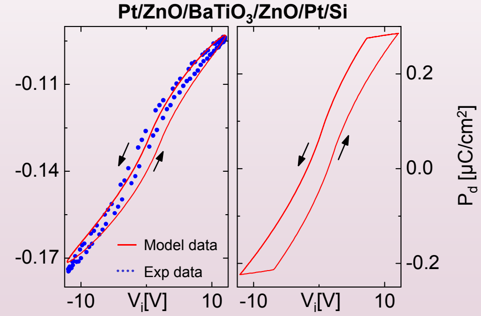
Pt/$BaTiO_3$/Pt/Si



Pt/ZnO/$BaTiO_3$/Pt/Si



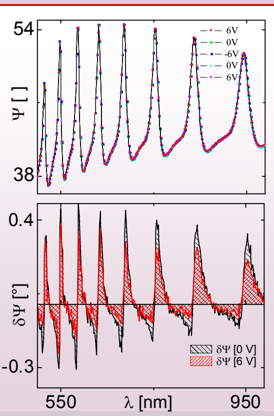
Pt/ZnO/$BaTiO_3$/ZnO/Pt/Si



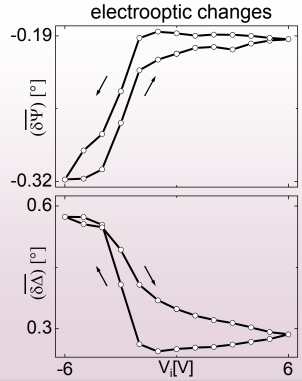
Best fit parameters

Pt/$BaTiO_3$/Pt/Si		Pt/ZnO/$BaTiO_3$/Pt/Si		Pt/ZnO/$BaTiO_3$/ZnO/Pt/Si	
R_s = 1 MΩ	P_s = 7.54 µC/cm²	R_s = 13 kΩ	P_s = 14.1 µC/cm²	R_s = 420 kΩ	P_s = 2 µC/cm²
ε_f = 202		ε_f = 250	P_r = 5.64 µC/cm²	ε_f = 60	P_r = 0.06 µC/cm²
E_c = 1.15 V/m	P_r = 1.39 µC/cm²	E_c = 1.1 V/m	P_{sz} = -4.1 µC/cm²	E_c = 1 V/m	P_{sz1}, P_{sz2} = 0.1µC/cm²

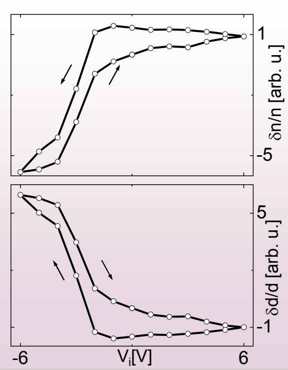
Electrooptic ellipsometry study of piezoelectric properties



Wavelength averaged electrooptic changes



Calculated data



Electrooptic ellipsometry difference spectra reveal effective (overall structure) index and thickness change hysteresis indicative for polarization coupling, and concordant with asymmetric electric and polarization hysteresis switching behavior.

The effective index and thickness changes are extracted from the electrooptic ellipsometry data by using the three phase model (ambient-film-substrate) [phys. stat. sol. (c) **5**, 1328 (2008)].

$$\begin{pmatrix} \frac{\delta n}{n} \\ \frac{\delta d}{d} \end{pmatrix} = \begin{pmatrix} S_{\delta\Psi}(n) & S_{\delta\Psi}(d) \\ S_{\delta\Delta}(n) & S_{\delta\Delta}(d) \end{pmatrix}^{-1} \begin{pmatrix} \delta\Psi \\ \delta\Delta \end{pmatrix}$$

The hysteresis behavior can be explained by the piezoelectric strain within the ferroelectric layer, by interface lattice charge coupling between the $BaTiO_3$ and ZnO layer, and the depletion layer formation within the n-type doped ZnO layer.

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