Electrooptic ellipsometry study of spontaneous polarization coupling in piezoelectric ZnO-BaTiO$_3$ heterostructures

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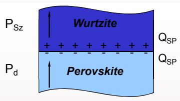
Polarization coupled interfaces



Is there a charge polarization coupling in BTO/ZnO?

Can this be used to determine the amount of the spontaneous polarization in ZnO?

We estimate the first experimental value for the spontaneous polarization in ZnO:
$P_{sz,\,ZnO}$ = - 4 µC/cm² [5]
Previous theory calculation: $P_{sz,\,ZnO}$ = - 5 ... - 5.7 µC/cm² [4]

[1] M. Schubert *et al.*, Ann. Phys. 13, 61 (2004);
[2] Mbenkum *et al.*, APL 86, 091904 (2005);
[3] Ashkenov *et al.*, Thin Solid Films 486 (2005) 153;
[4] Bernardini *et al.*, PRB 56, R10024 (1997)
[5] V. M. Voora *et al.*, J. Electron. Mater, XX, XXXX (2007).

➢The coupling between the non-switchable lattice charge of wurtzite structure (ZnO) and the switchable ferroelectric polarization P_s in perovskite structure (BaTiO$_3$) is interesting [1,2].

➢Here we report on electrical [3] and electrooptic measurements of Pt/BaTiO$_3$/ZnO/Pt heterostructures.

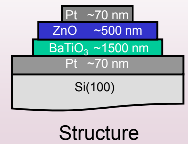
➢We observe index of refraction and piezoelectric thickness hysteresis behavior concordant with electrical polarization hysteresis.

➢The simulations to the right depict electric Sawyer-Tower and BTO polarization hysteresis loops for our ZnO/BTO heterostructure. The model parameters are listed below.

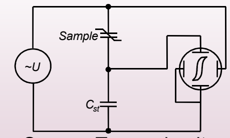
Experiment

➢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.



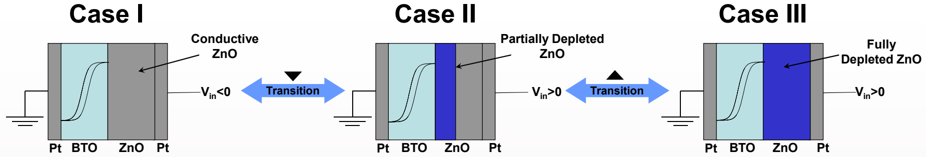
Structure



Sawyer-Tower circuit

Electric interface polarization coupling and depletion layer model

Case I   Case II   Case III



Case I:

$$V = E_f d_f.$$

$$V = \sigma_b \frac{d_f}{\varepsilon_f} - P_d \frac{d_f}{\varepsilon_f} - P_{sz} \frac{d_z}{\varepsilon_z}.$$

Case II:

$$V = \frac{eN_c w^2}{2\varepsilon_z} - E_f d_f.$$

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

$$eN_c w + P_{sz} = E_f \varepsilon_f + P_d.$$

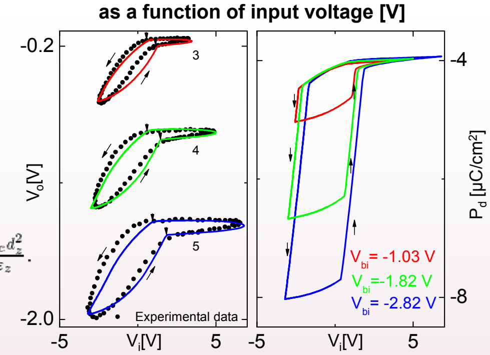
Case III:

$$V = E_z d_z - \frac{eN_c d_z^2}{2\varepsilon_z} + E_f d_f.$$

$$V = \sigma_b \left(\frac{d_f}{\varepsilon_f} + \frac{d_z}{\varepsilon_z}\right) - P_d \frac{d_f}{\varepsilon_f} - P_{sz} \frac{d_z}{\varepsilon_z} + \frac{eN_c d_z^2}{2\varepsilon_z}.$$

$$eN_c d_z + E_z \varepsilon_z + P_{sz} = E_f \varepsilon_f - P_d.$$

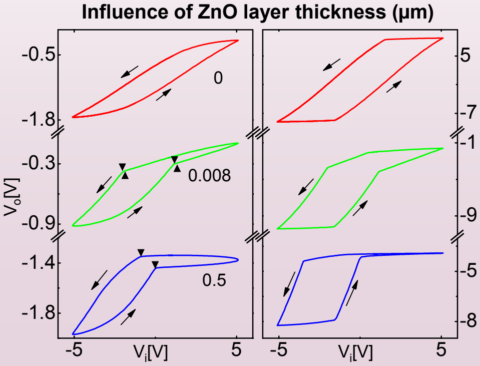
Experimental and model calculated data as a function of input voltage [V]



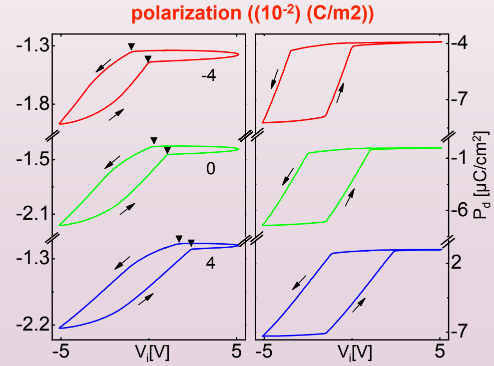
Best fit Sawyer-Tower model parameters

Thickness of BaTiO$_3$ (d_z)	0.5		µm
Thickness of ZnO (d_f)	1.45		µm
Input frequency (f)	1.5		kHz
Sample resistance (R_s)	13		kΩ
Dielectric constant of BaTiO$_3$ (ε_{BTO})	250		
Dielectric constant of ZnO (ε_{ZnO})	8		
Coercive field (E_c)	1.2	$\times 10^6$	V/m
Saturation polarization (P_s)	14.1		µC/cm²
Remanent polarization (P_r)	6.35		µC/cm²
Intrinsic concentration in ZnO (N_c)	5.5	$\times 10^{22}$	m^{-3}
Built-in voltage with in the sample(V_{bi})	----		V
spontaneous polarization in ZnO (P_{sz})	-4.0		µC/cm²

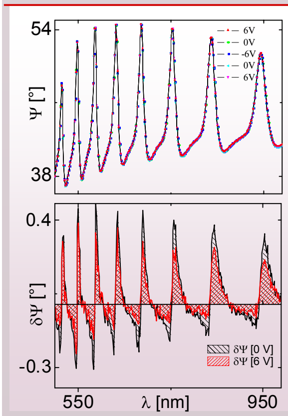
Influence of ZnO layer thickness (µm)



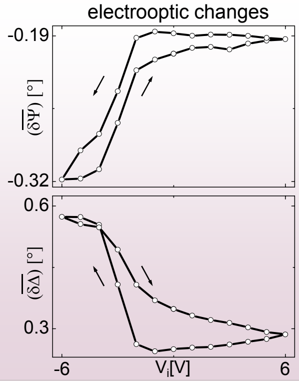
Influence of ZnO spontaneous polarization ((10^{-2}) (C/m2))



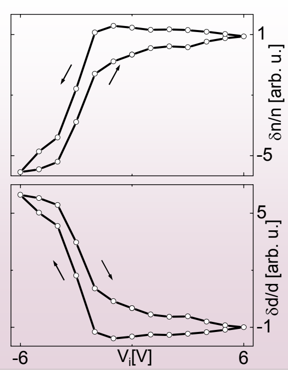
Electrooptic ellipsometry study of piezoelectric properties



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 ellipsometrye data by using the three phase model (ambient-film-substrate) [6].

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

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.

[6] V. M. Voora, *et al.*, *Phys. Status Solidi C* XX, XXXX (2008)

RESEARCH FAIR , UNL, April 2, 2008

Support: DFG FOR 404, UNL Startup, NSF MRSEC, JAWF