Electrooptic ellipsometry study of spontaneous polarization coupling in piezoelectric ZnO-$BaTiO_3$ heterostructures

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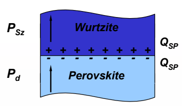
Polarization coupled interfaces



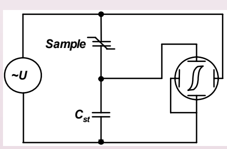
Is there a charge polarization coupling in BTO/ZnO?

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

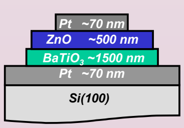
ZnO is a wurtzite structure typically n-type semiconductor with ionic interface charge (spontaneous polarization P_{sz}). This charge interacts with the switchable (ferroelectric) perovskite structure polarization P_s in BTO. This coupling influences the BTO index of refraction [1], the ferroelectric phase transition [2], and the rectifying electrical properties of ZnO/BTO heterostructures. We previously predicted that this coupling can be used to determine P_{sz} of ZnO. Here we report on electrical and electrooptic measurements of Pt/BTO/ZnO/Pt heterostructures, and our new model approach, in which we included the effect of a charge depletion layer in ZnO. We observe index of refraction and piezoelectric thickness hysteresis behavior concordant with electrical polarization hysteresis. From analysis of our data:

We estimate the first experimental value for the spontaneous polarization in ZnO:
$P_{sz,\,ZnO}$ = - 4 μC/cm² [ICSE4]
Previous theory calculation: $P_{sz,\,ZnO}$ = - 5 ... - 5.7 μC/cm² [4]

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

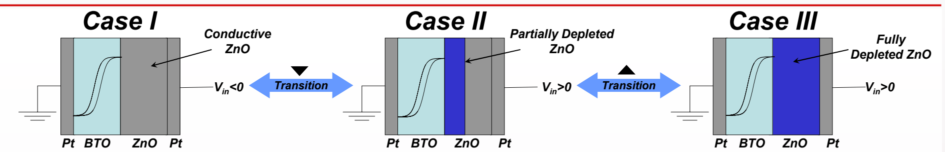


Samples are prepared by Pulsed Laser Deposition, and subsequent masking with ohmic Pt back and front contacts. Electric and electrooptic ellipsometry measurements were performed on contacts and near contacts, respectively.



[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)

Electric interface polarization coupling and depletion layer model



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:

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

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

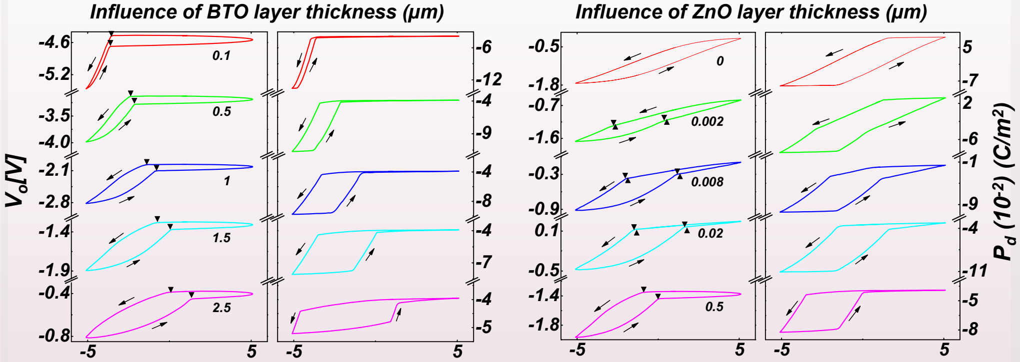
$$eN_c w + P_{sz} = E_f \varepsilon_f + P_d$$

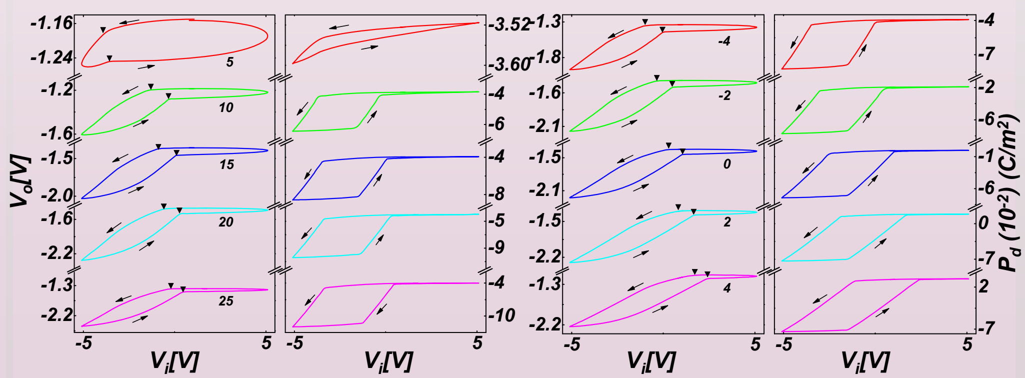
Case III:

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

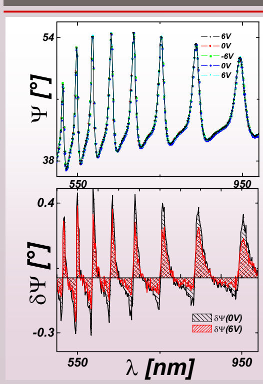
$$V = \sigma_b \left(\frac{d_f}{\varepsilon_f} + \frac{d_z}{\varepsilon_z} \right) - P_d \frac{d_f}{\varepsilon_f} - P_{sz} \frac{d_z}{\varepsilon_z} + \frac{eN_c d_z^2}{2\varepsilon_z}$$

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

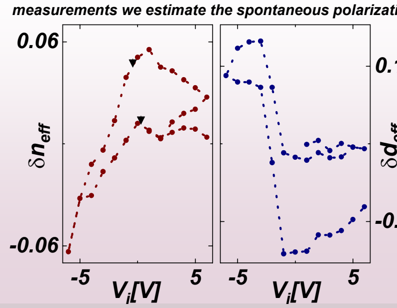


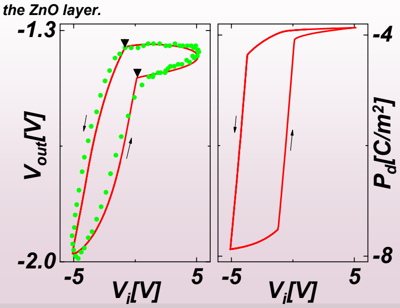


Electrooptic ellipsometry and Sawyer Tower Circuit analysis



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. From best-fit model analysis of Saywer-Tower circuit measurements we estimate the spontaneous polarization in the ZnO layer.





N_c = 5.5×10²² /m³
ε_{BTO} =250
ε_{ZnO} =8
E_c =1.2×10⁶ V/m
P_s =14.1×10⁻² C/m²
P_r =6.35×10⁻² C/m²
P_{sz} =-4.0×10⁻² C/m²
R_s =13 kΩ

Best fit Sawyer-Tower model parameters

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