Conduction Band Offset and Polarization Effects in InAs Nanowire Polytype Junctions

I-Ju Chen, Sebastian Lehmann, Malin Nilsson, Pyry Kivisaari,
Heiner Linke, Kimberly A. Dick, and Claes Thelander

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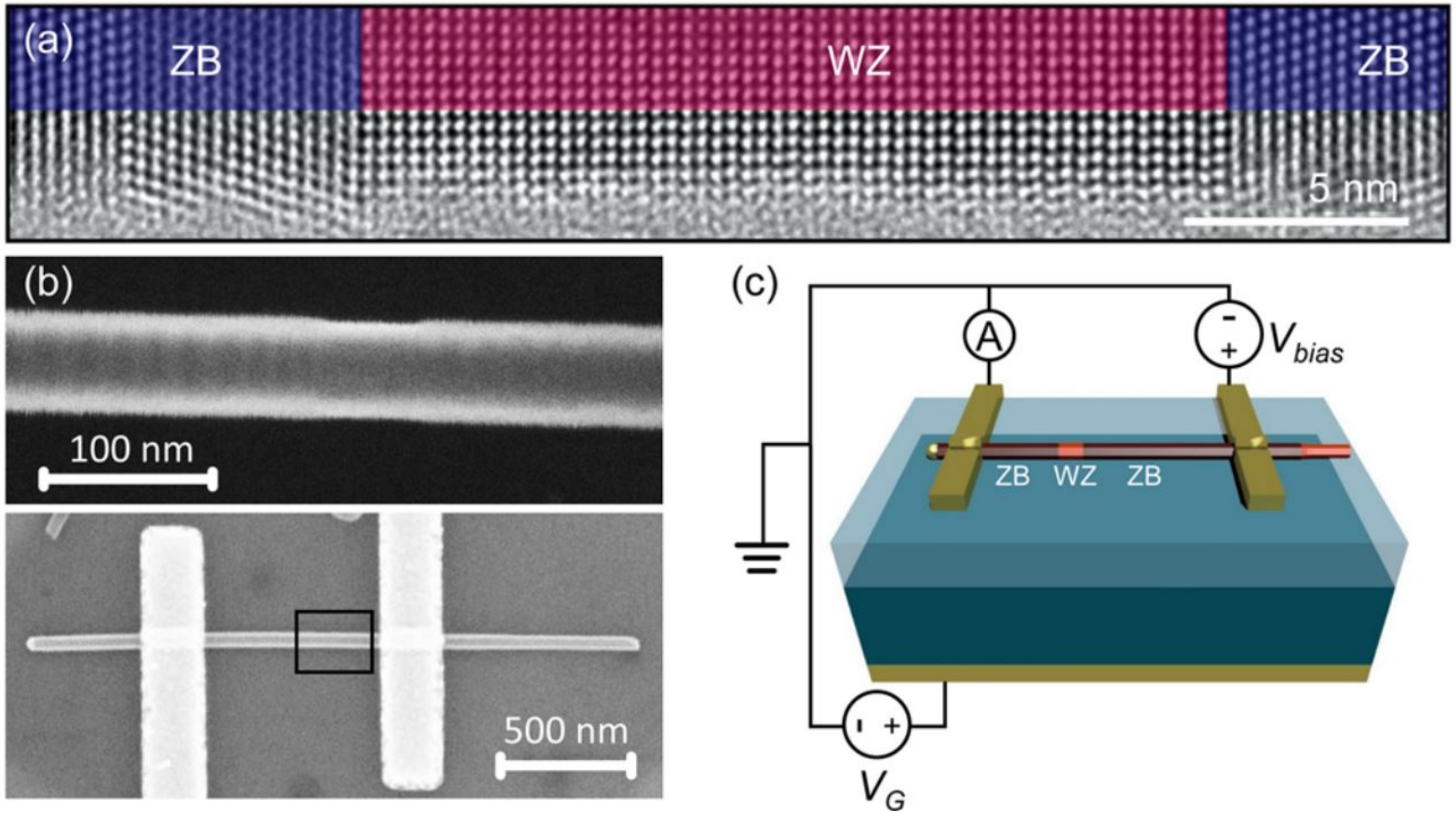
Motivation

- InAs are used in quantum transport studies such as conductance quantization, spin manipulation and quantum computing
- Grown InAs nanowires suffer from a high density of stacking defects or polytypism
- Here: zinc blende (ZB) and wurzite (WZ)
- Theroy shows that WZ has a larger bandgap than ZB with an up to 126 meV positive conduction band offset
- Currently unclear, how polytypism affects electron transport properties

Device

- Wires grown by low pressure MOVPE
- Change in AsH3 molar fractions results in two crystal structures (ZB and WZ)
- 2 terminal device with backgate
- Junction: ZB-WZ-ZB
- WZ with different lengths: 8, 19, 45, 82, 210 nm
- 60 ± 5 nm in diameter, WZ slightly less thick (< 3 nm)



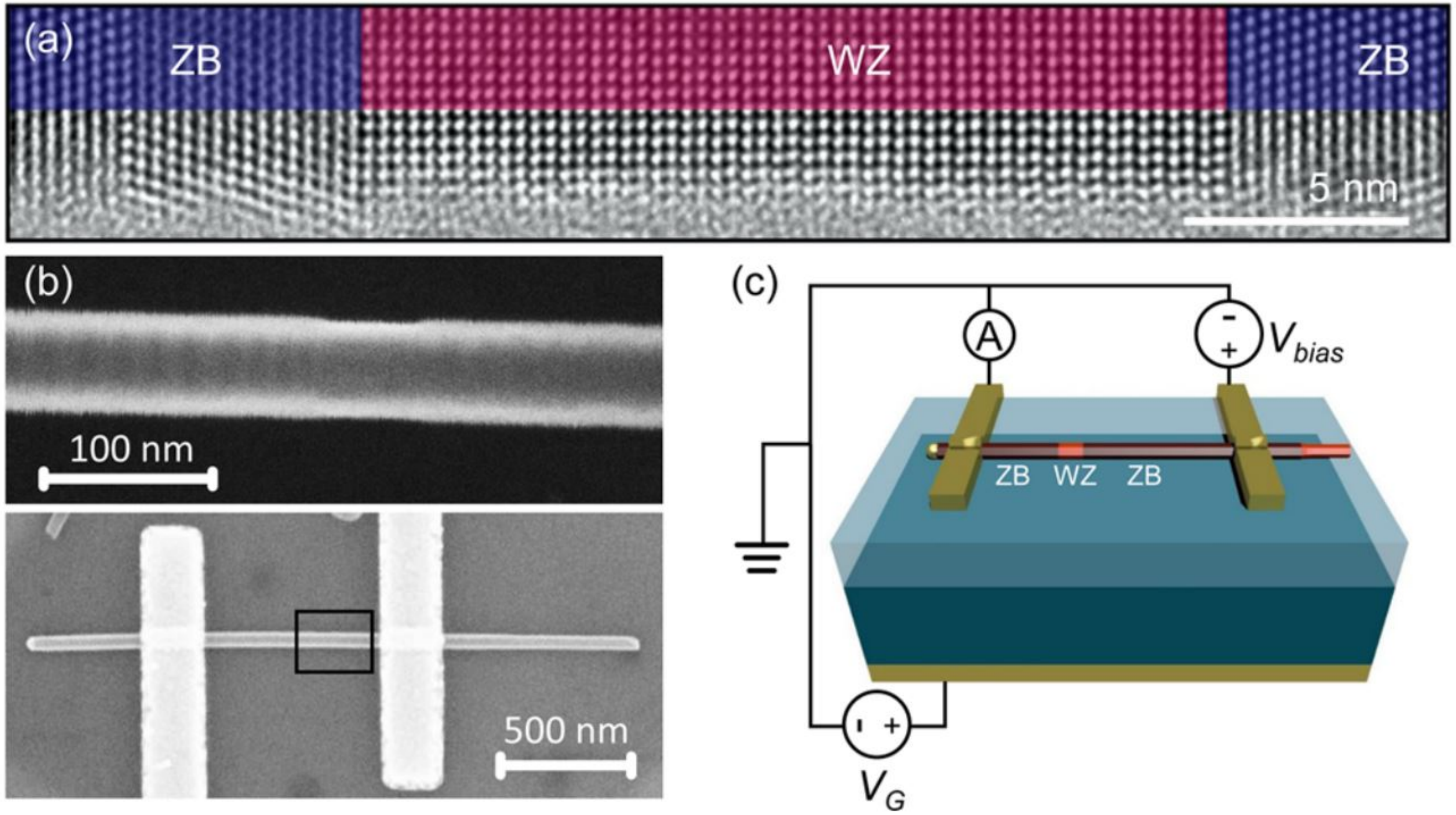
- Difference in carrier concentration

$$n_{\mathrm{ZB}} = 2.6 \cdot 10^{18}\ \mathrm{cm}^{-3},$$
$$n_{\mathrm{WZ}} = 5.7 \cdot 10^{17}\ \mathrm{cm}^{-3}$$

- Difference in mobility

$$\mu_{\mathrm{ZB}} = 3000\ \mathrm{cm}^2\mathrm{V/s},$$
$$\mu_{\mathrm{WZ}} = 2500\ \mathrm{cm}^2\mathrm{V/s}$$

- Lower symmetry of WZ crystal phase
  - Spontaneous polarization field
  - Polarization charges at the interface between WZ an ZB



Electrical Characterization

- Temperature dependent $I - V_{\text{bias}}$ curves 110 K < T < 240 K

- Rate-limiting process: thermionic emission

Activation energy

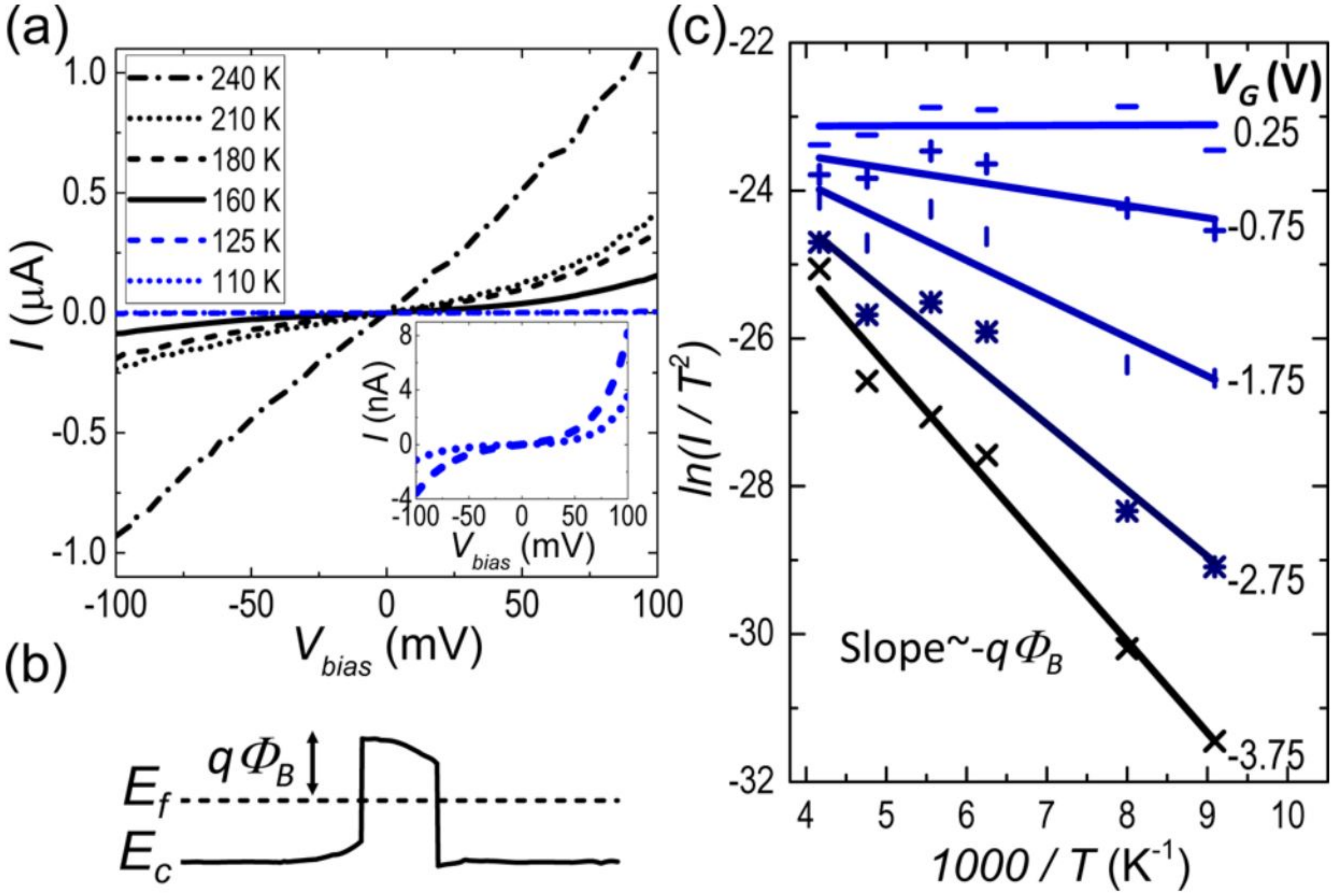
Current density

$$J = A T^2 exp\left(-\frac{q\Phi_B}{k_B T}\right)$$

Richardson's constant

- Activation energy: difference between conduction band edge at the top of the WZ barrier and the Fermi level E_{f}

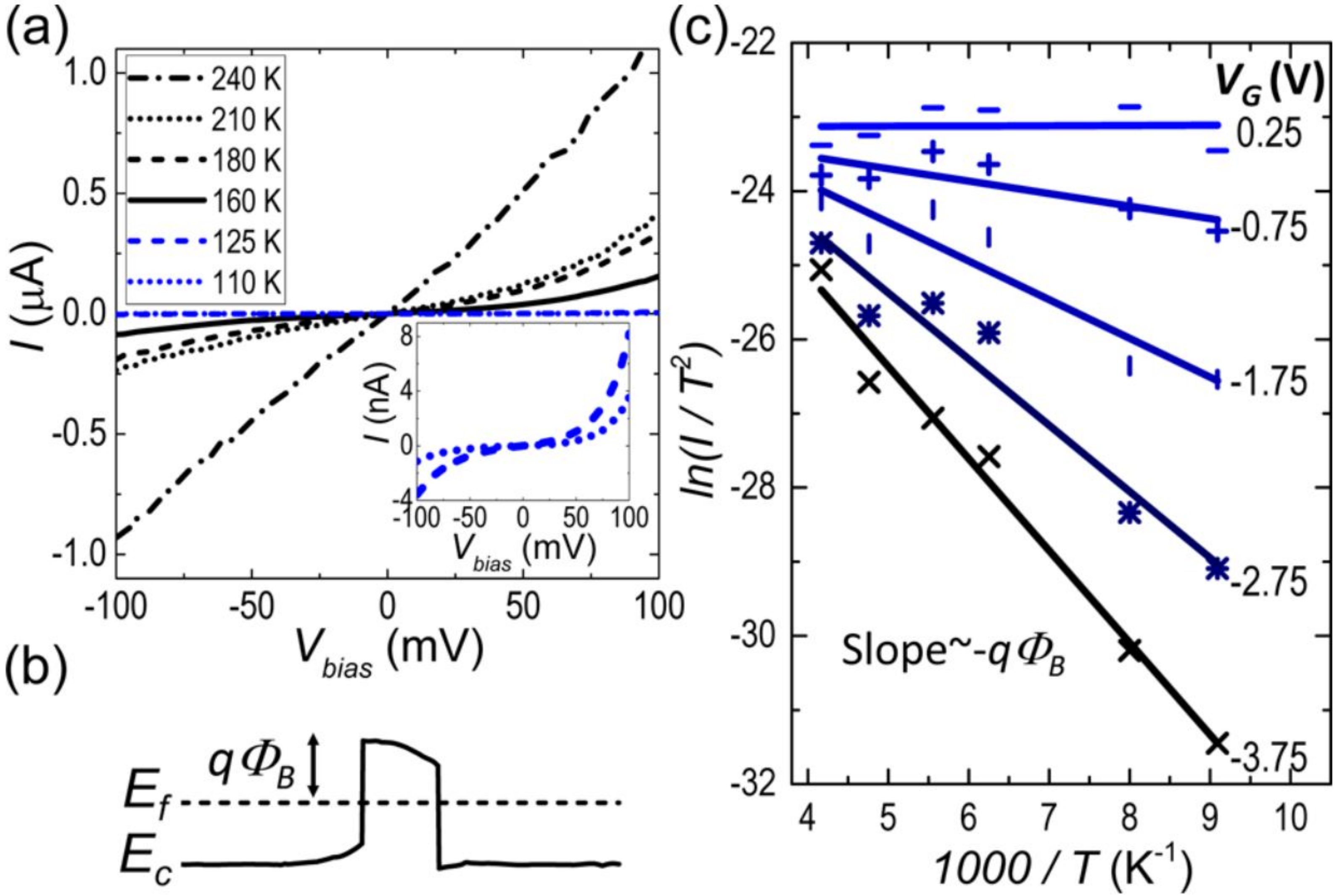
- Can be obtained by fitting the temperature-current relation



Electrical Characterization

$$J = A\ T^2 exp\left(-\frac{q\Phi_B}{k_B T}\right)$$

- Only valid for nondegenerate barriers, i.e., when $q\Phi_B \gg k_B T$
- For $q\Phi_B < 0$, E_f is in conduction band
  - ➢ No longer limited by thermionic emission due to absence of an activation barrier
- Note the small asymmetry in the I-V curves



Carrier Concentration

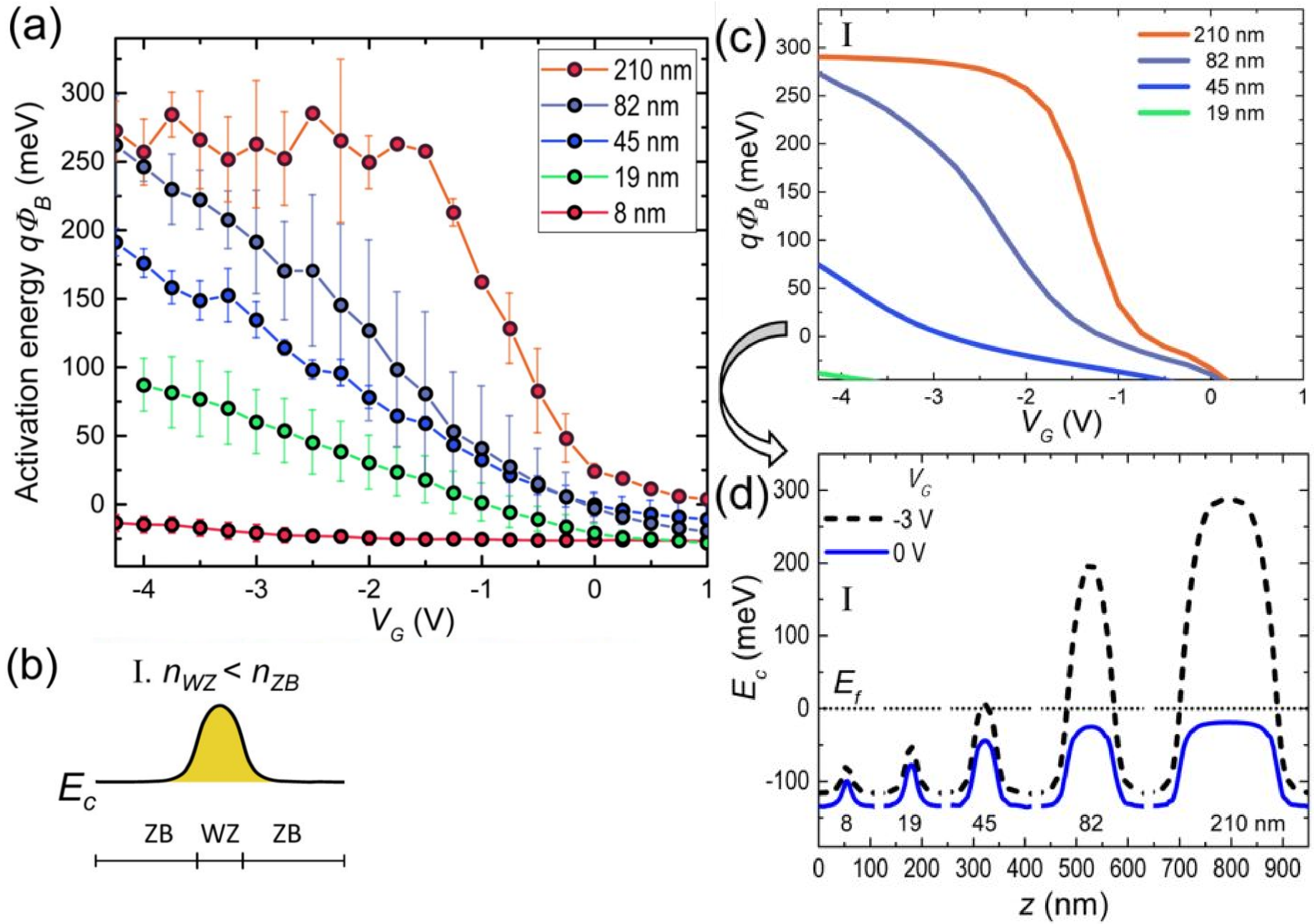
- Increase of $q\Phi_B$ with segment length L_{WZ}

- Suggests that lower carrier concentration influences the formation of the potential barriers

- Simulations (using only carrier concentration) reproduce the increasing trend (but do not represent short WZ segments)

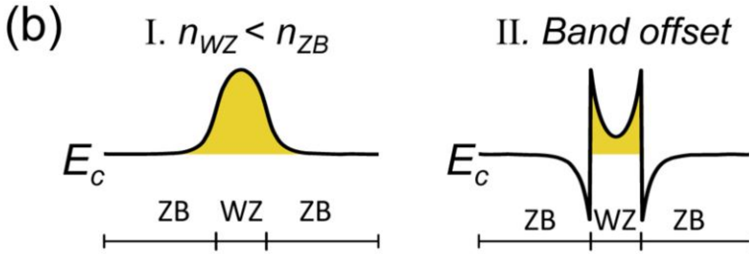
- For short WZ segments, carrier diffusion lowers barrier energy
  - ➢ No significant potential barrier

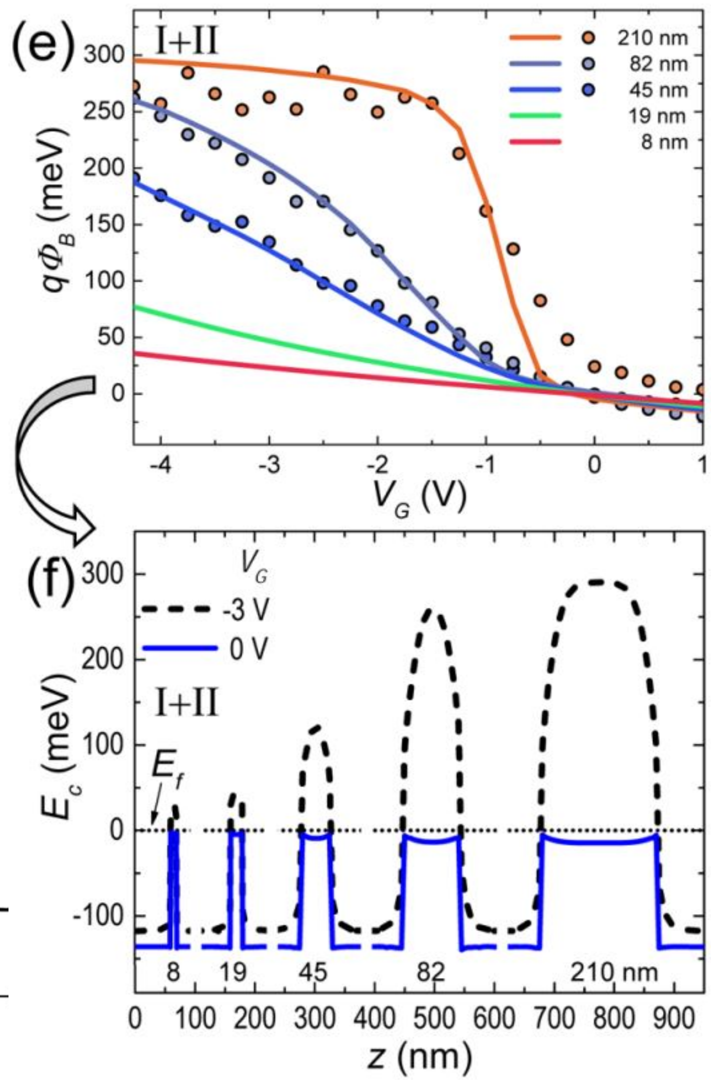
- Barrier height is sensitive to WZ length and relative carrier concentrations across the interface -> depends on V_G



Band Offset

- Introducing a positive offset of the conduction band minima of InAs WZ
- Fitted the measured values of $q\Phi_B$ by varying WZ band gap, conduction band offset and surface donor state density in ZB and WZ
- Band offset (86 - 126 meV) reduces the carrier diffusion at interface
  - ➢ buildup of energy barriers
- Calculated band gap smaller than measured, model does not include tunneling in valence band (underestimation of the band gap)
- Footnote: STS measurements do not yield any band offset...





Polarization Charge

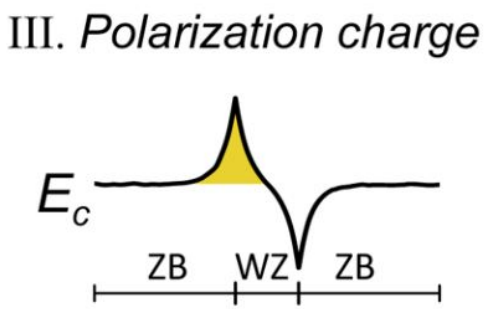
- In WZ crystals the tetrahedron is commonly distorted
  - ➢ Spontaneous polarization P_{sp}

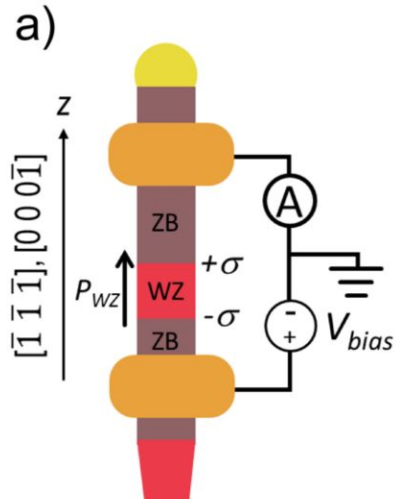
- Additionally, strain gives rise to piezoelectric polarizations P_{pz}

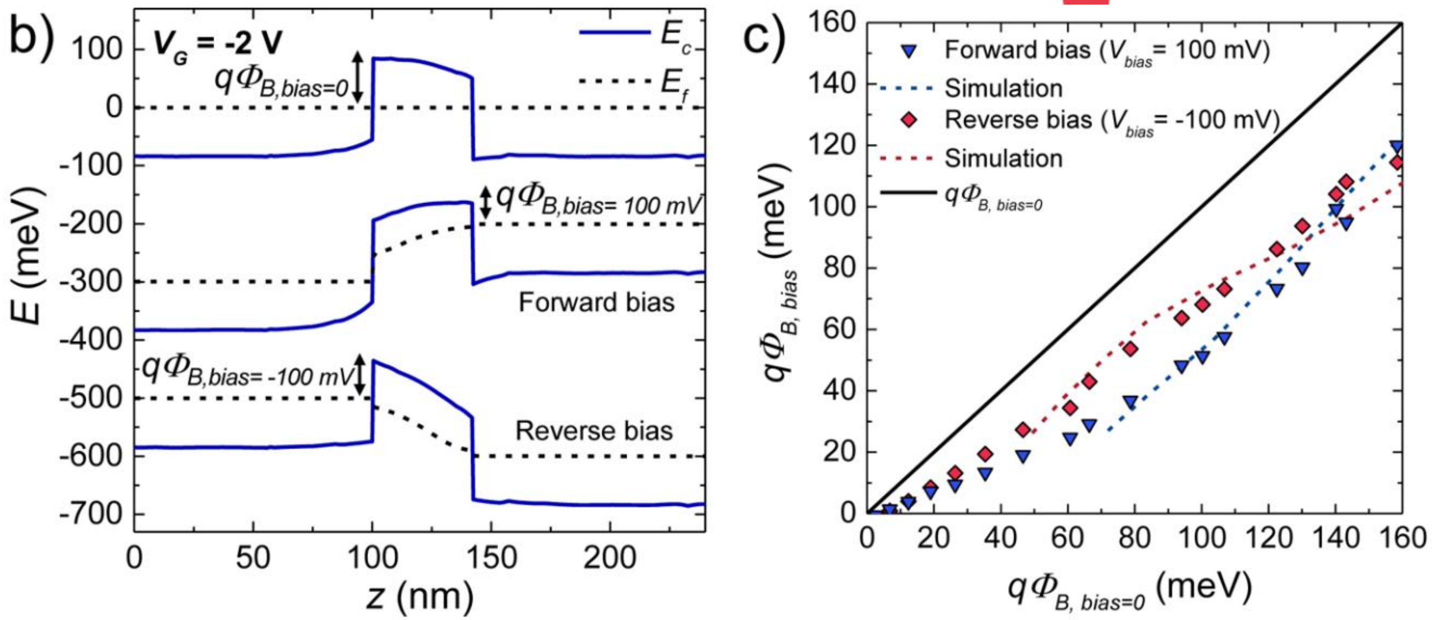
- This results in a polarization field related to the polarization charge density σ

$$\delta P = \delta(P_{\mathrm{sp}} + P_{\mathrm{pz}}) = -\sigma$$

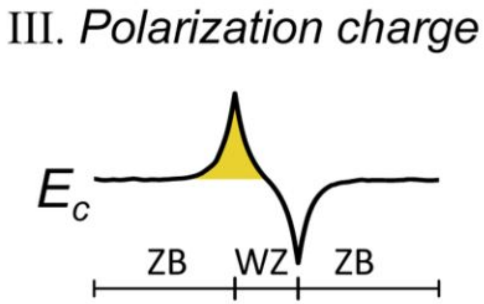
- Abrupt change in polarization field leads to an accumulation or depletion of electrons
  - ➢ Asymmetric potential

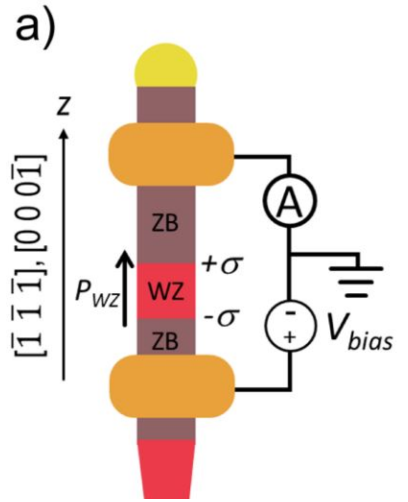


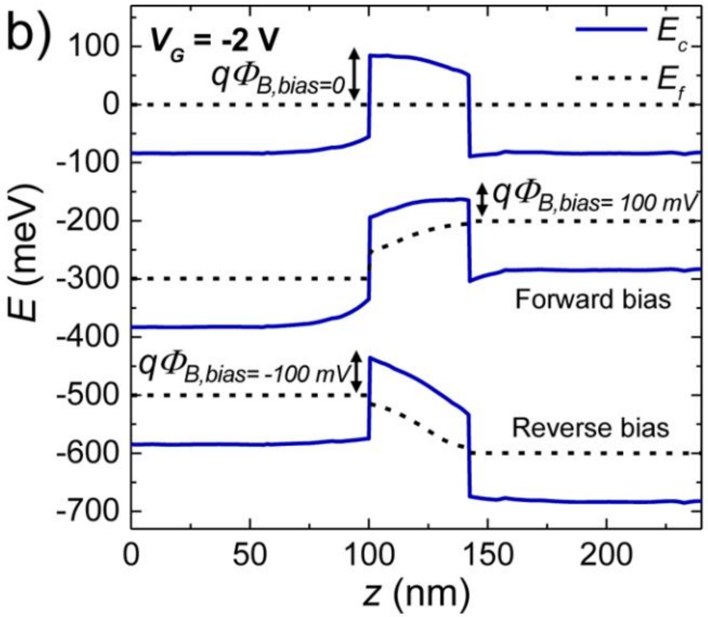


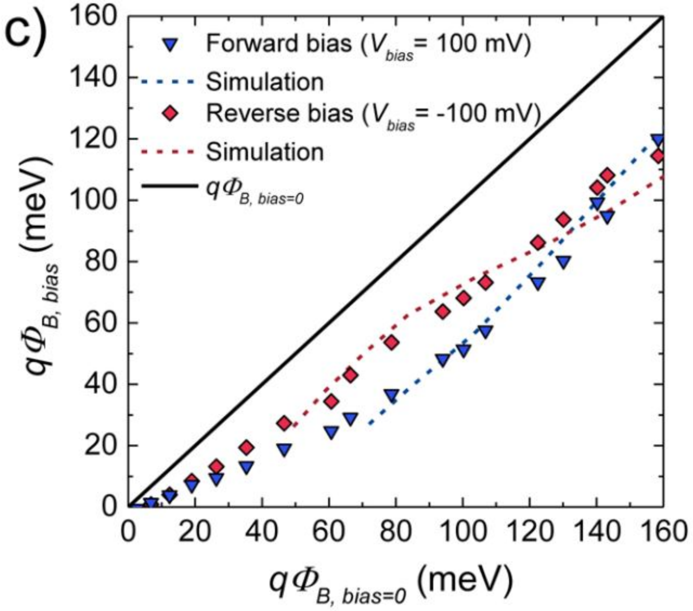


- Asymmetry can be seen in measurements of different bias polarities
- Positve polarization charge at the top results in accumulation of electrons
- Slight current rectification can be reduced by choosing the bias properly



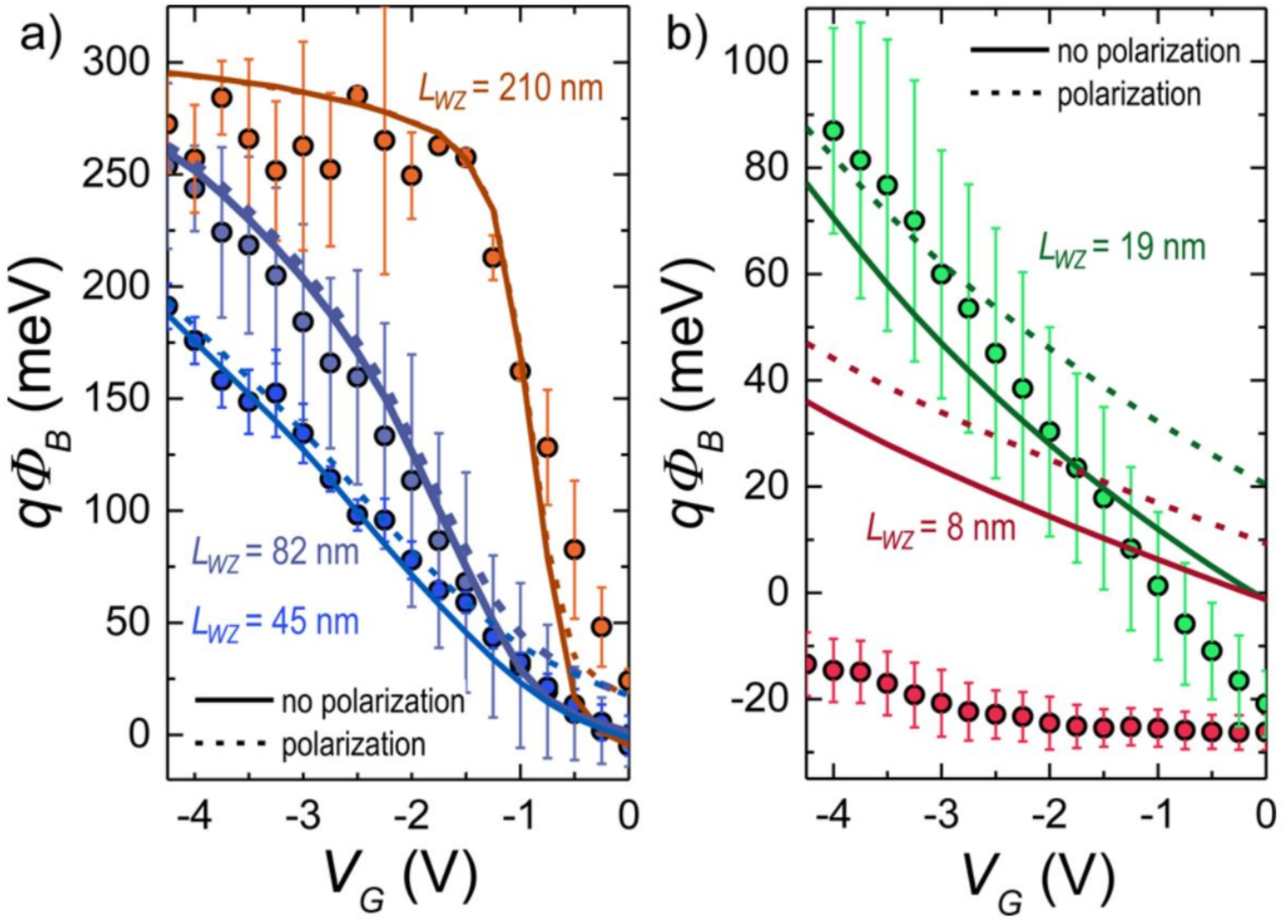






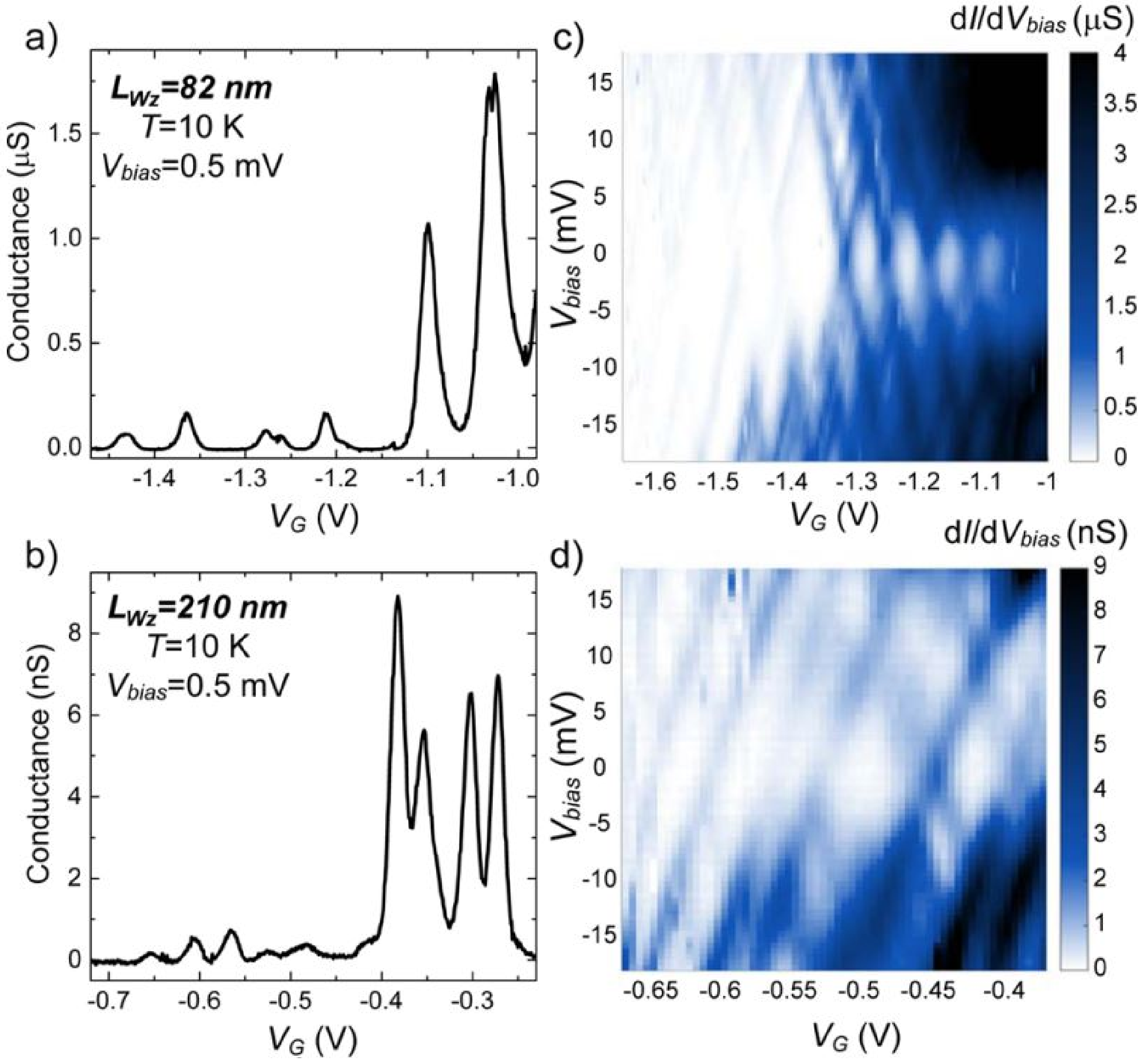
Adding All Up

- Extracted polarization charge σ is included in simulation of V_G-dependent $q\Phi_B$
- Raise of activation energy values (obvious for shorter L_{WZ})
- Measured activation energy still lower than calculated (for shorter L_{WZ})
  - Electron tunneling as main contribution



Quantum Dots

- Due to the band offset it should be possible to form a shallow quantum dot within a WZ segment
- Low temperature (10 K ...) measurements were performed
- Both 82 and 210 nm WZ segments showed Coulomb oscillations and Coulomb blockade diamond patterns
- Shorter ones did not show any periodic oscillations
- Shows the presence of a band offset on both interfaces



Summary

- Effect of polytypism on the electronic properties was studied
- Based on controlled ZB-WZ-ZB junctions
- Understand and differentiate the roles of
  1. Carrier concentration
  2. Band offset and
  3. Interfacial polarization charge
- Conduction band discontinuity results in abrupt energy barriers at each interface
- Can be used as tunnel barriers for quantum dot experiments

➢ Better predictions for the electronic properties and improvements for existing band structure models