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Interpretation of scanning tunneling spectroscopy of semiconductor nanostructures

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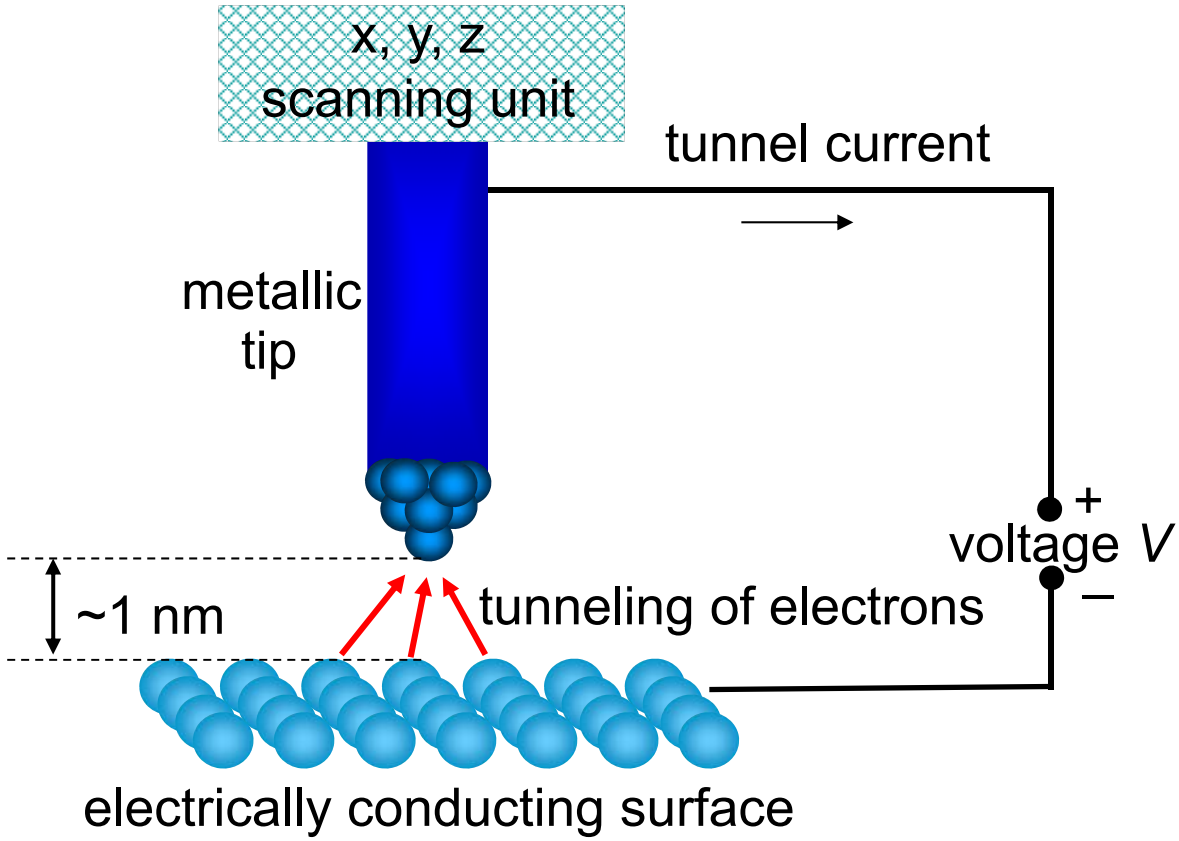
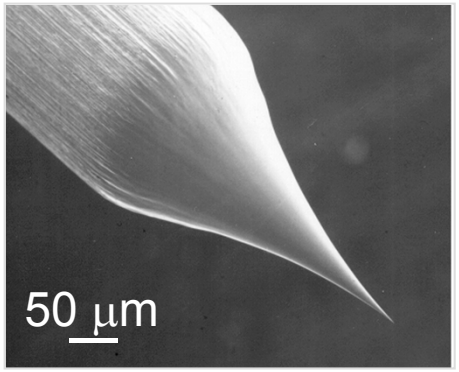
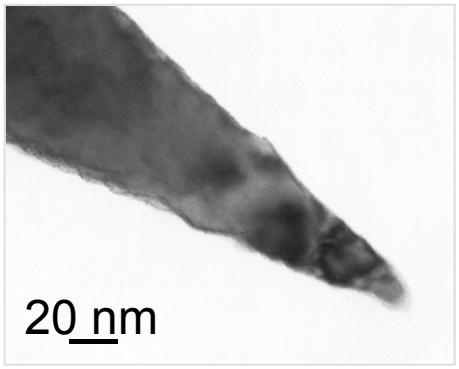
The scanning tunneling microscope

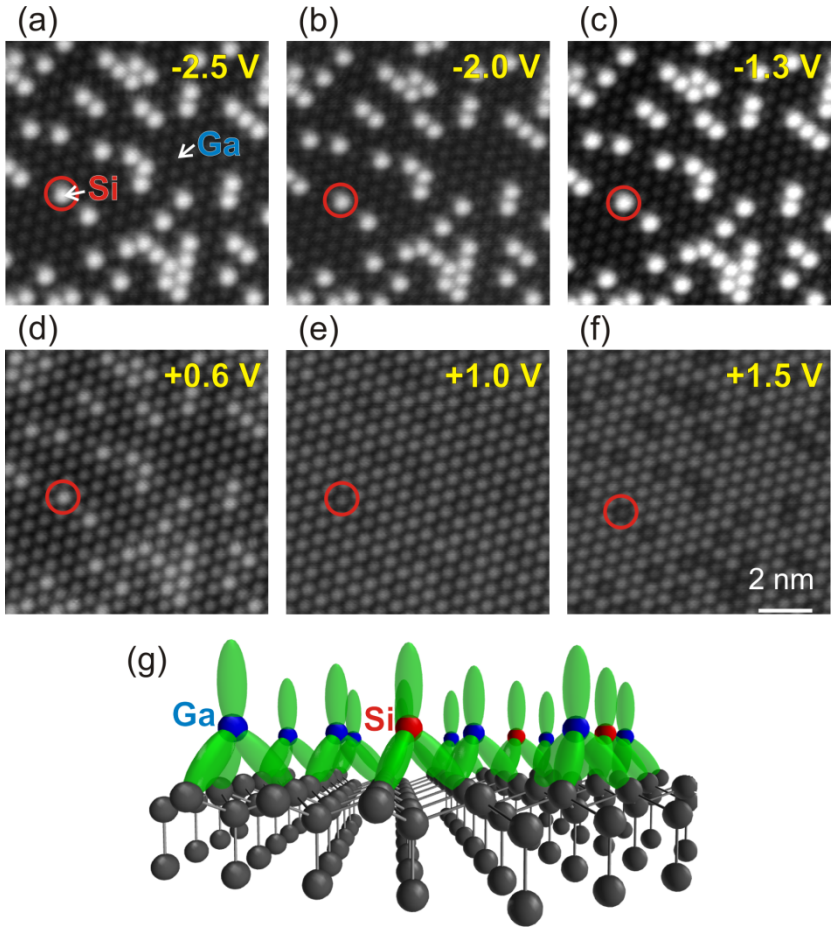


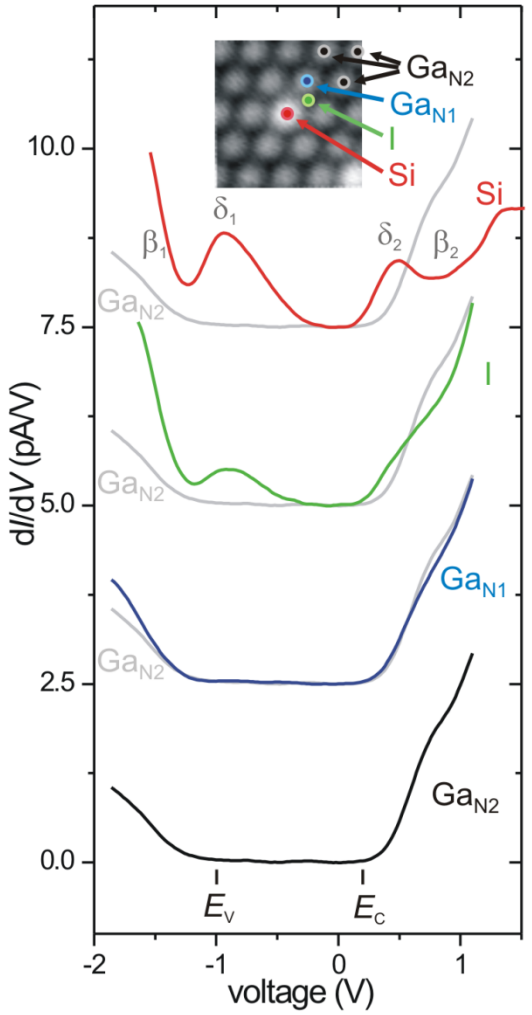
tunneling tip





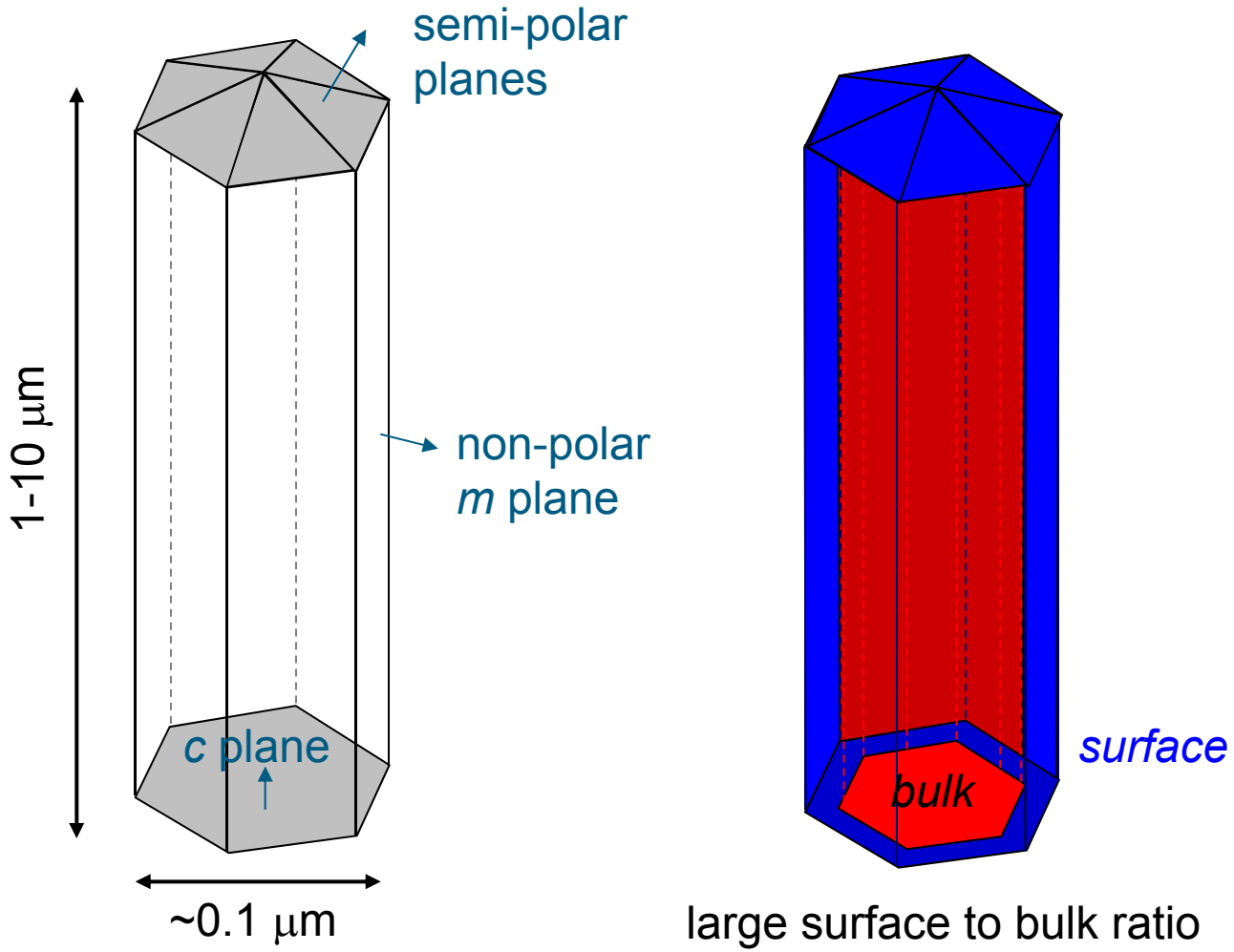
Scanning tunneling spectroscopy





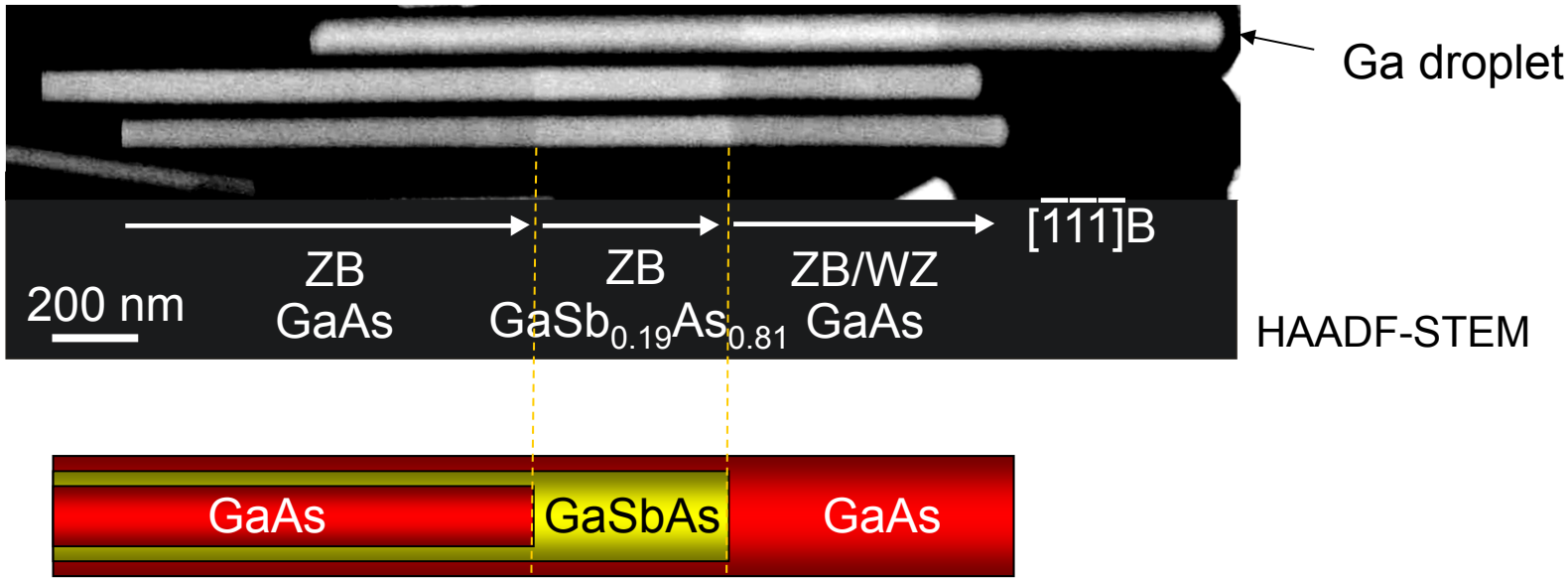
Ebert *et al.*, Nano Lett. **12**, 5845 (2012)

Nanowires: relevance of surfaces



large surface to bulk ratio
surface dominates NWs properties

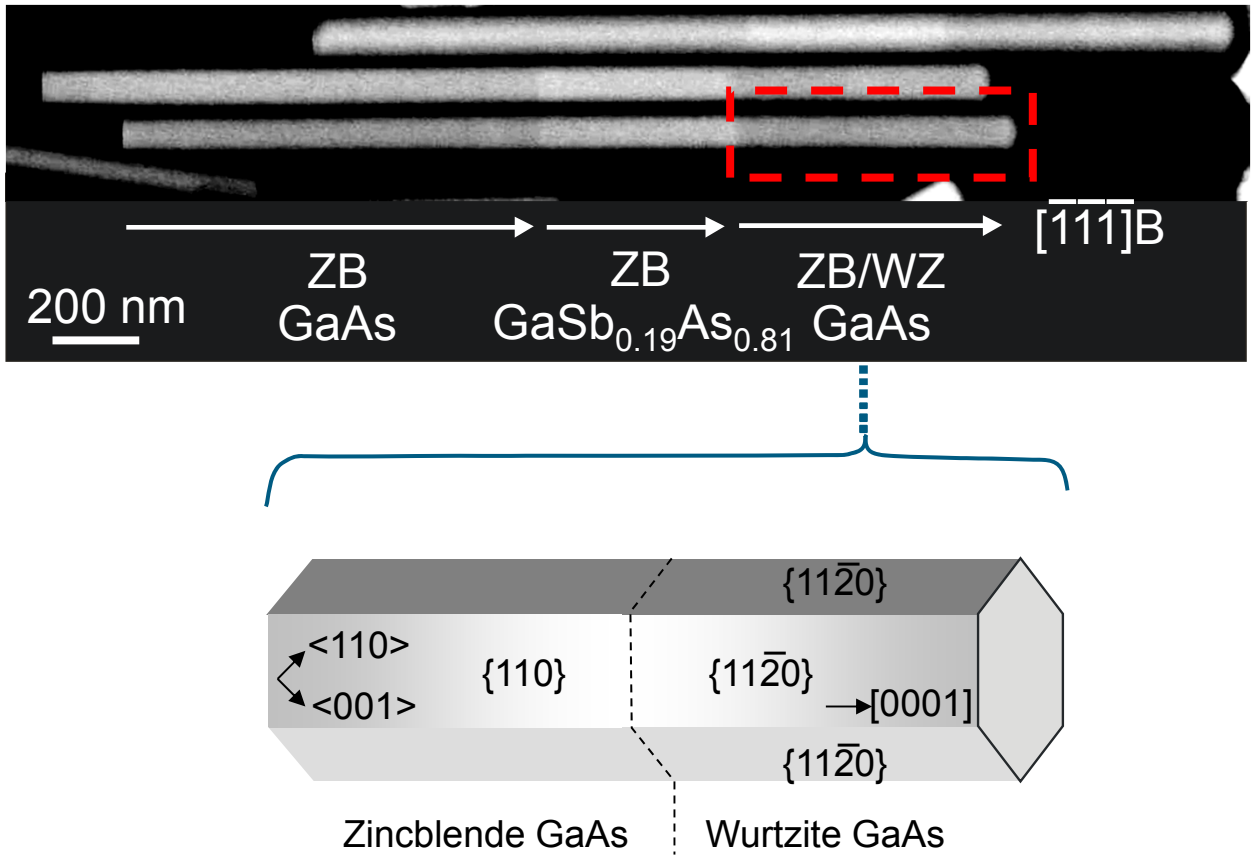
GaAs/$GaAs_{0.81}Sb_{0.19}$/GaAs NW heterostructures



- undoped GaAs NWs
- solid source MBE; 630°C
- Ga assisted; Ga, As_4 and Sb_2 fluxes 0.25, 0.50, and 0.66 ML/s
- self-overgrowth GaAs/$GaAs_{0.81}Sb_{0.19}$/GaAs NW heterostructures
- nucleated on native oxide-covered Si(111)

Growth: see Plissard *et al.*, APL **96**, 121901 (2010).

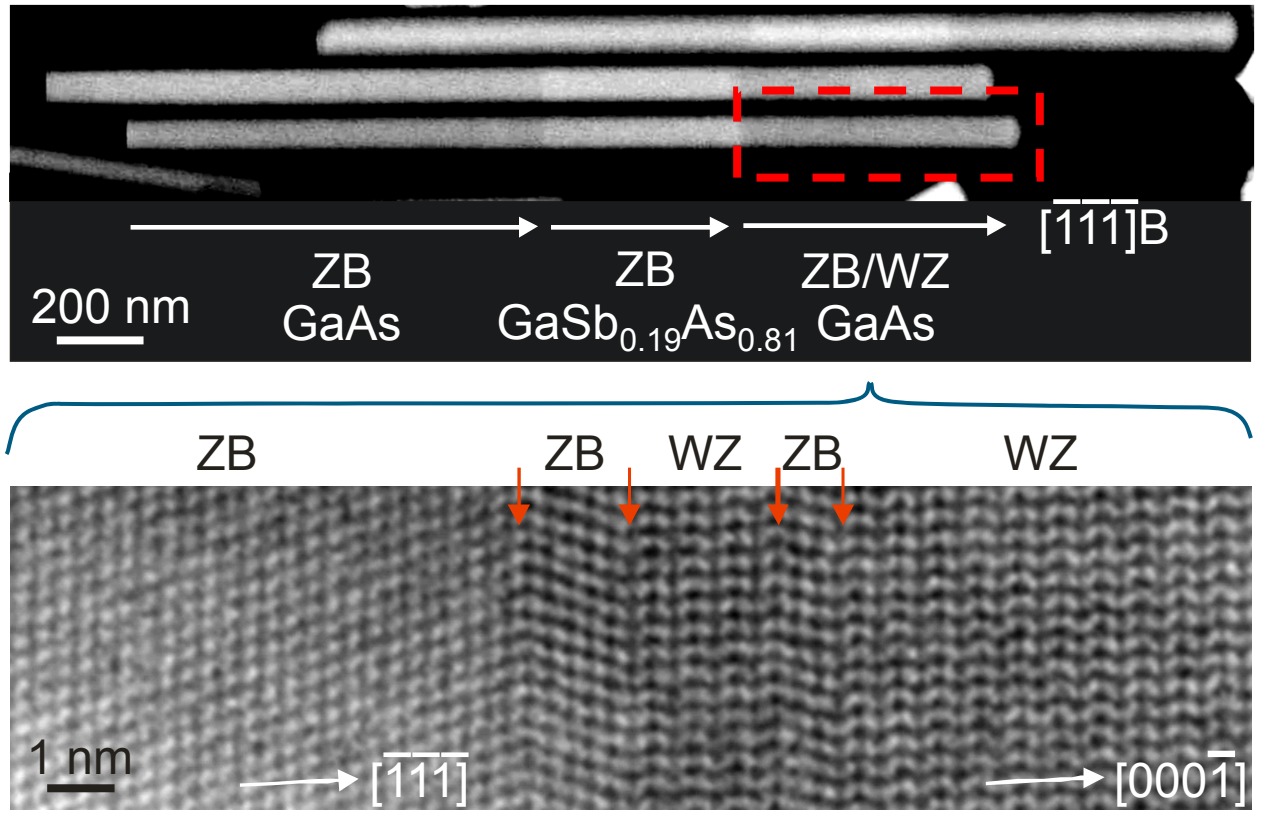
Top GaAs segment: ZB-WZ interface



HAADF-STEM

Capiod *et al.*, APL **103**, 122104 (2013)

Top GaAs segment: ZB-WZ interface



HAADF-STEM

Zincblende-Wurtzite Structure transition
with several twin boundaries/stacking faults

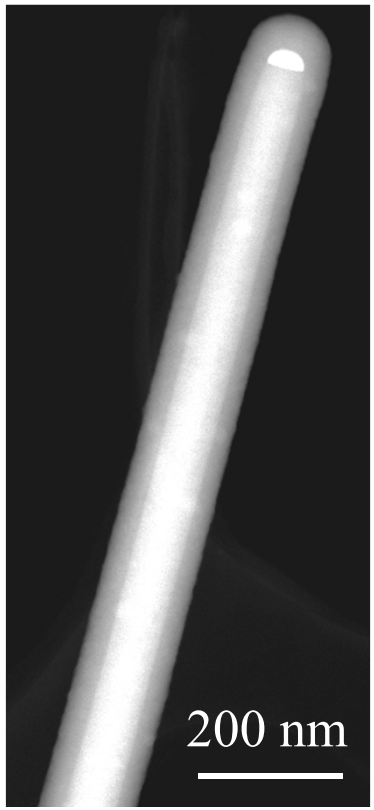
Capiod *et al.*, APL **103**, 122104 (2013)

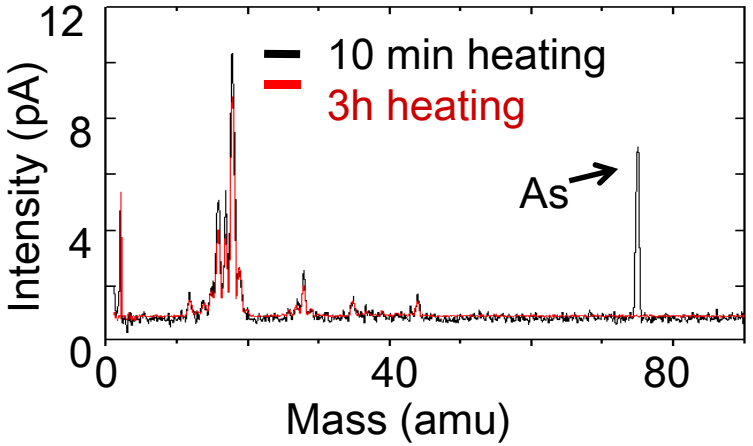
Preparation for STM

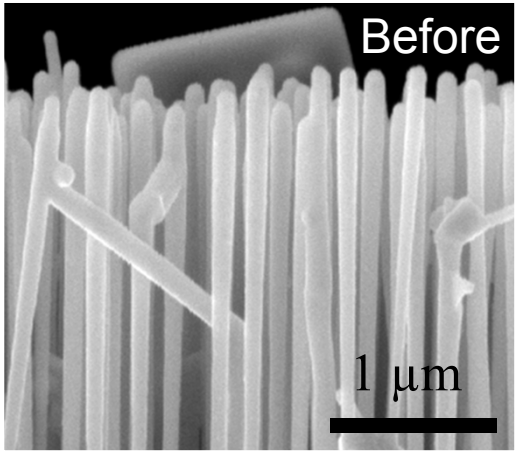
- NWs capped with a thin As layer at end of growth:
  T=300 K, 50 min high As_4 flux: protection against oxidation.
- Full consumption of Ga droplet
- In STM system: capping layer desorbed in-situ at 350°C for 4 h
- $p<1x10^{-10}$ mbar

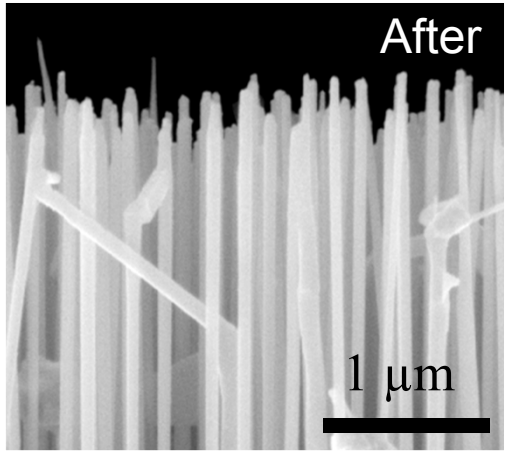
For details see: Xu *et al*., Nanotechnology **23**, 095702 (2012)

As decapping



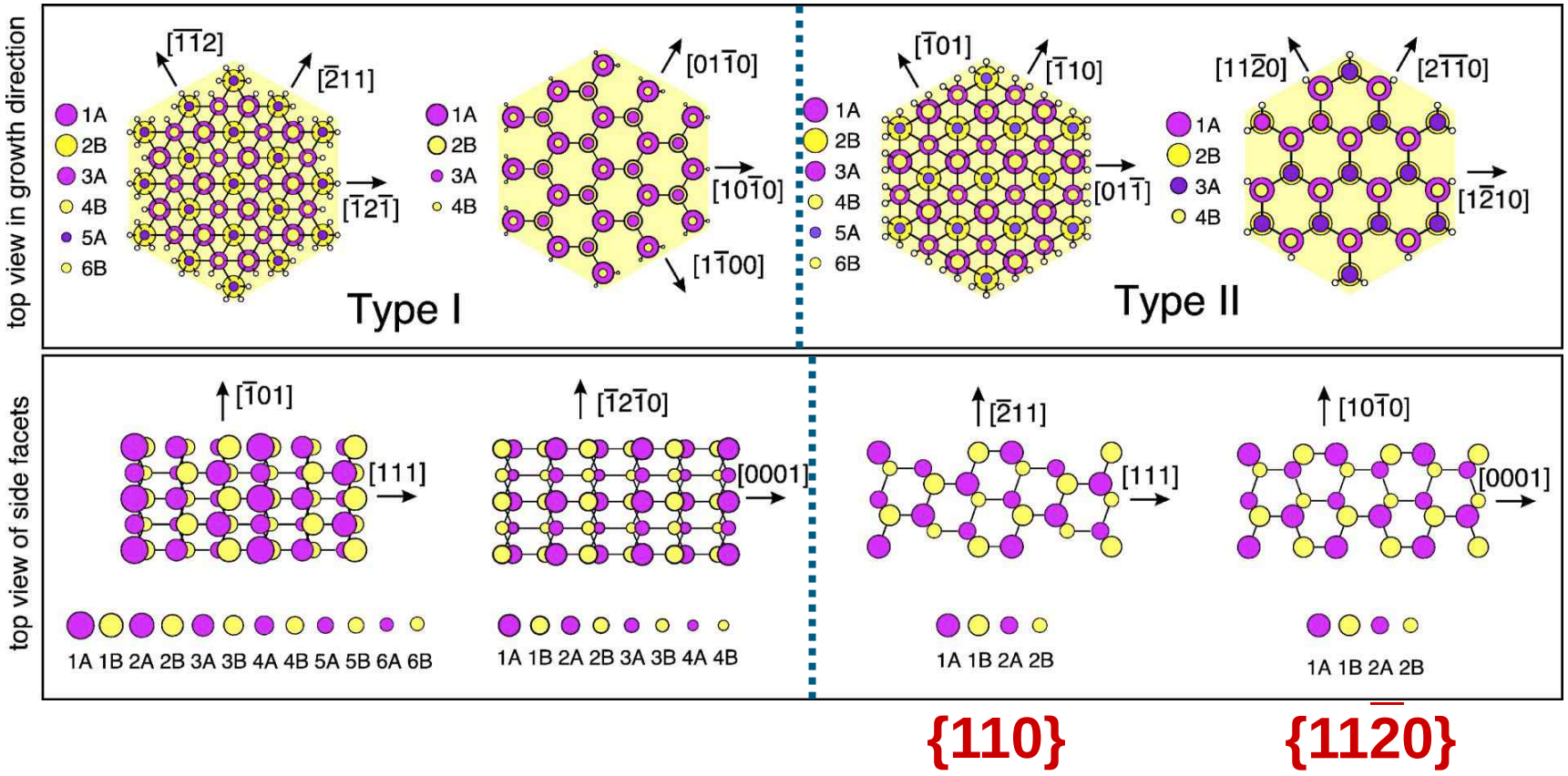






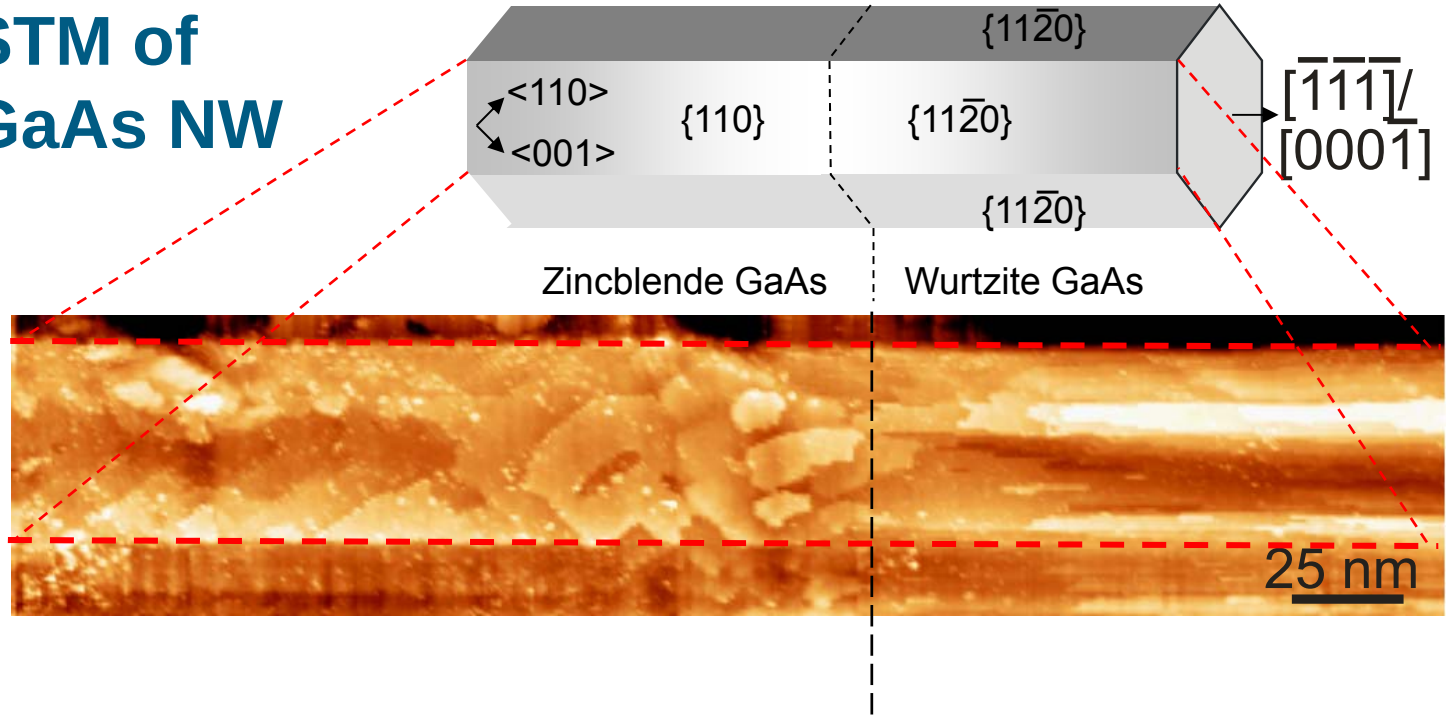
- Cleaving off the NWs on a degenerately doped 7x7 Si(111) surface
- Cleaved-off NWs lie flat on Si(111) substrate: imaging by STM, 77 K

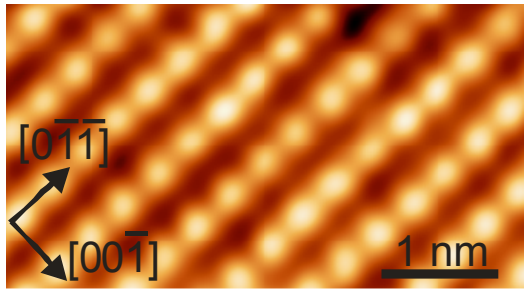
Geometrical structure of the GaAs NW

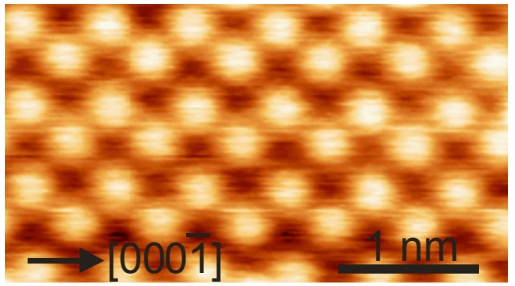


Leitsmann & Bechstedt, JAP **102**, 063528 (2007)

STM of GaAs NW







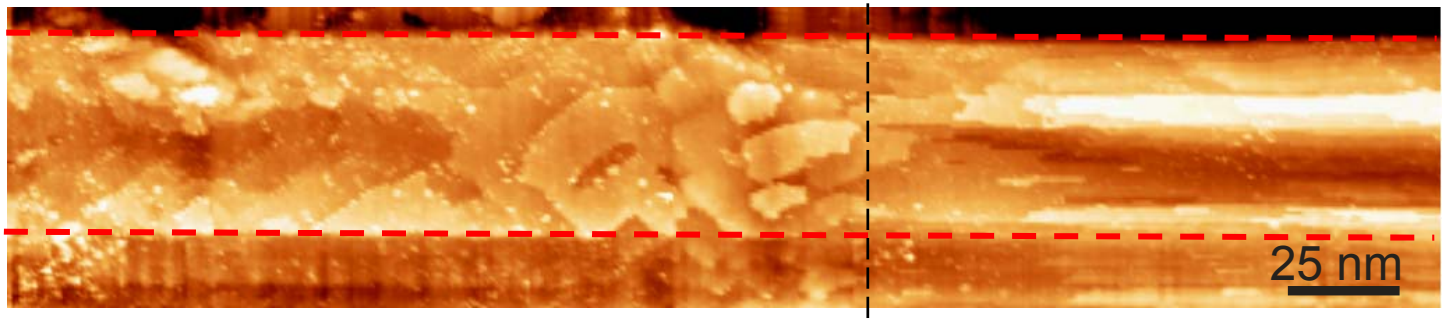
ZB GaAs(0$\bar{1}$1)

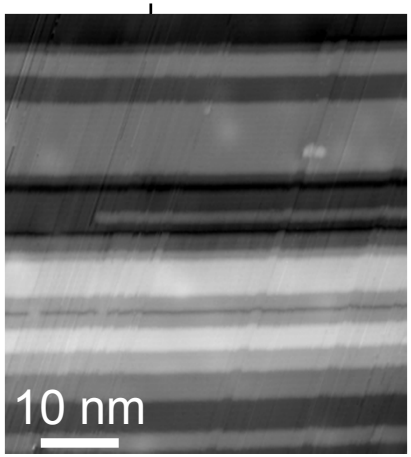
WZ GaAs(11$\bar{2}$0)

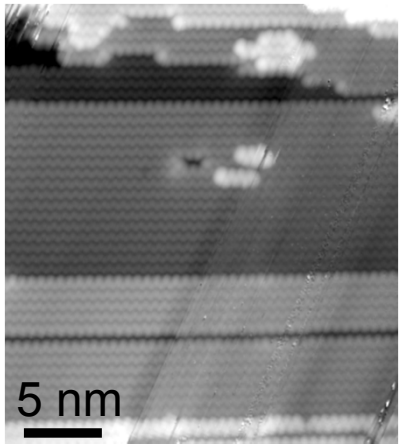
Capiod *et al.*, APL **103**, 122104 (2013)

Step structure on NW sidewall surfaces

WZ GaAs(11$\bar{2}$0)





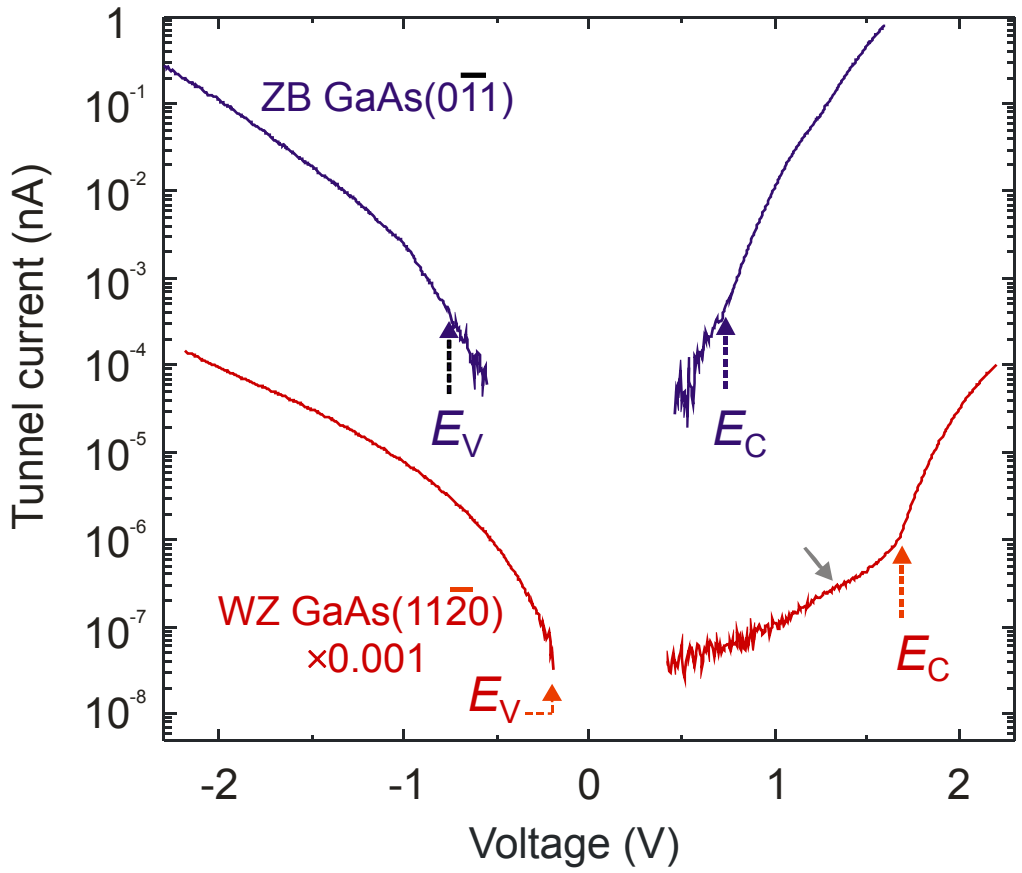


High step densities:

ZB: steps along <110>, <001>
WZ: steps along [0001]

CdSe (11$\bar{2}$0): Siemens *et al.*, PRB **59**, 3000 (1999).

Scanning tunneling spectroscopy: ZB and WZ sections

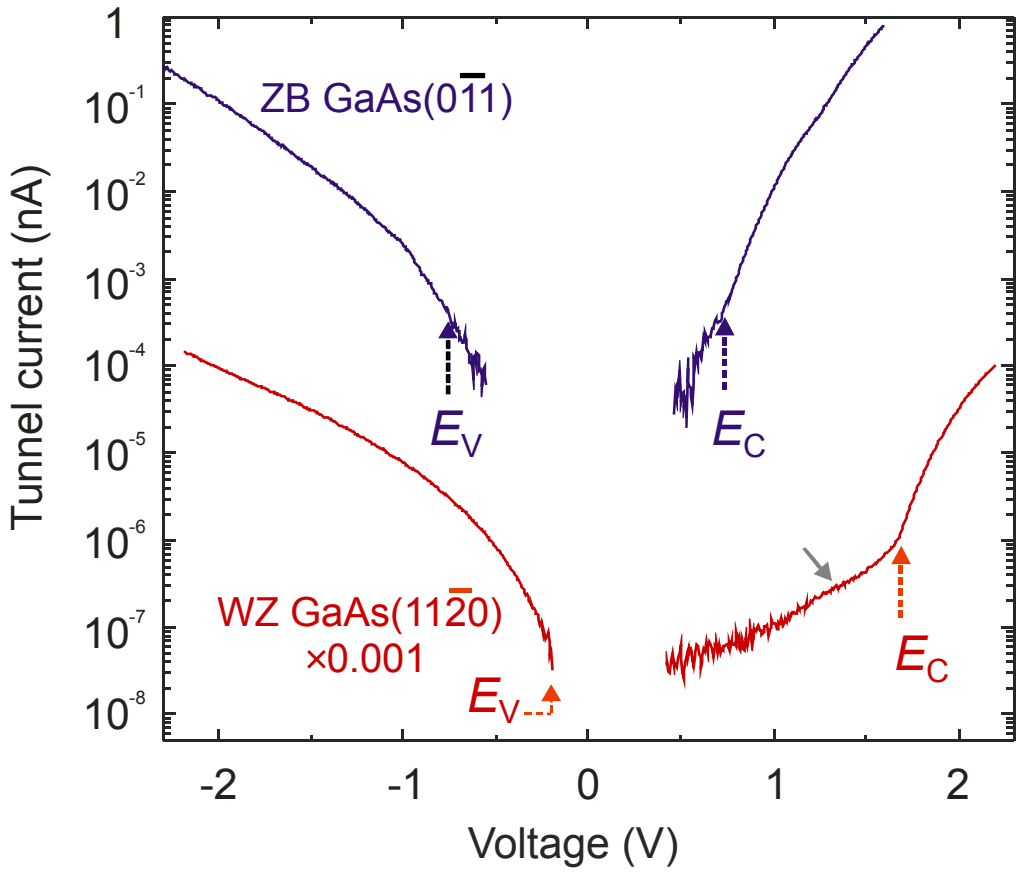


Capiod *et al.*,
APL **103**, 122104 (2013)

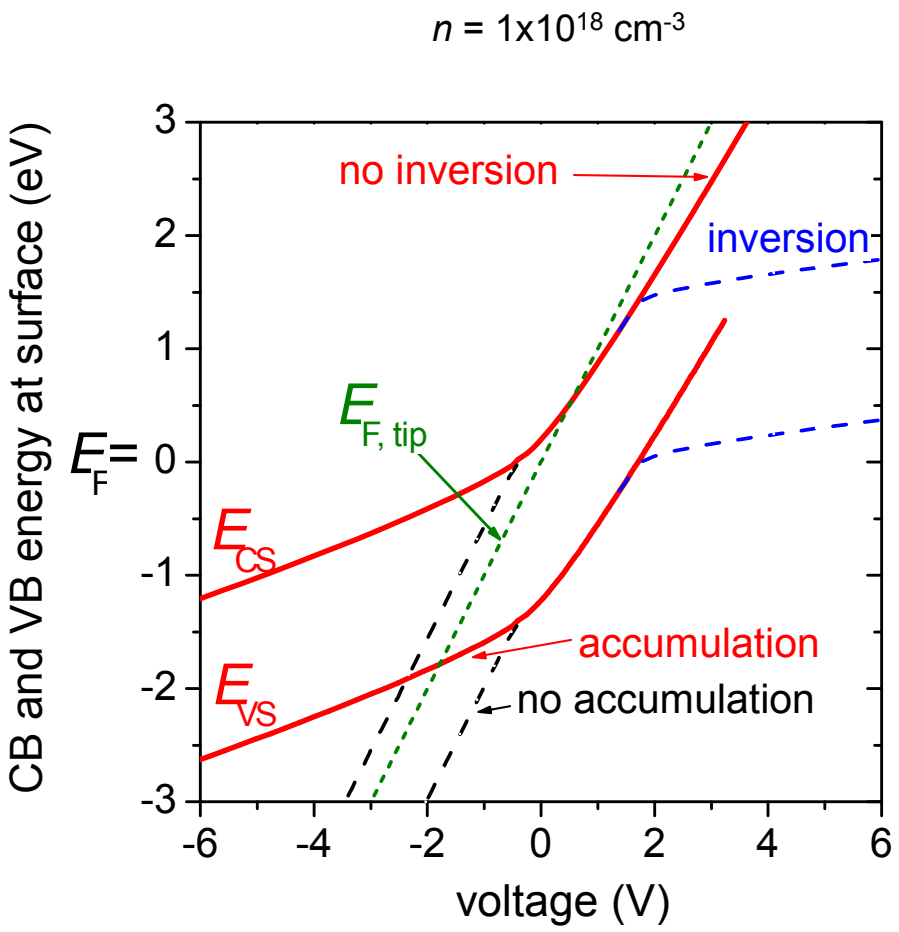
Band edges? Band gaps?

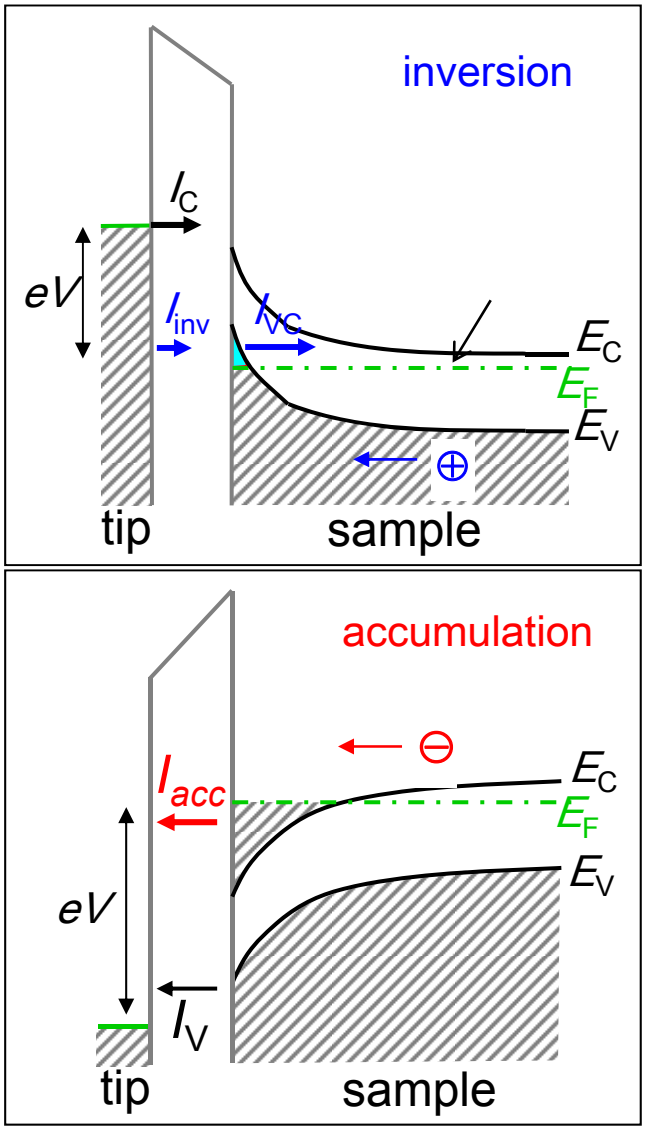
How to interpret STS?
Band edges? Band gaps?

- undoped GaAs NW
- high step densities
- STM: surface probe



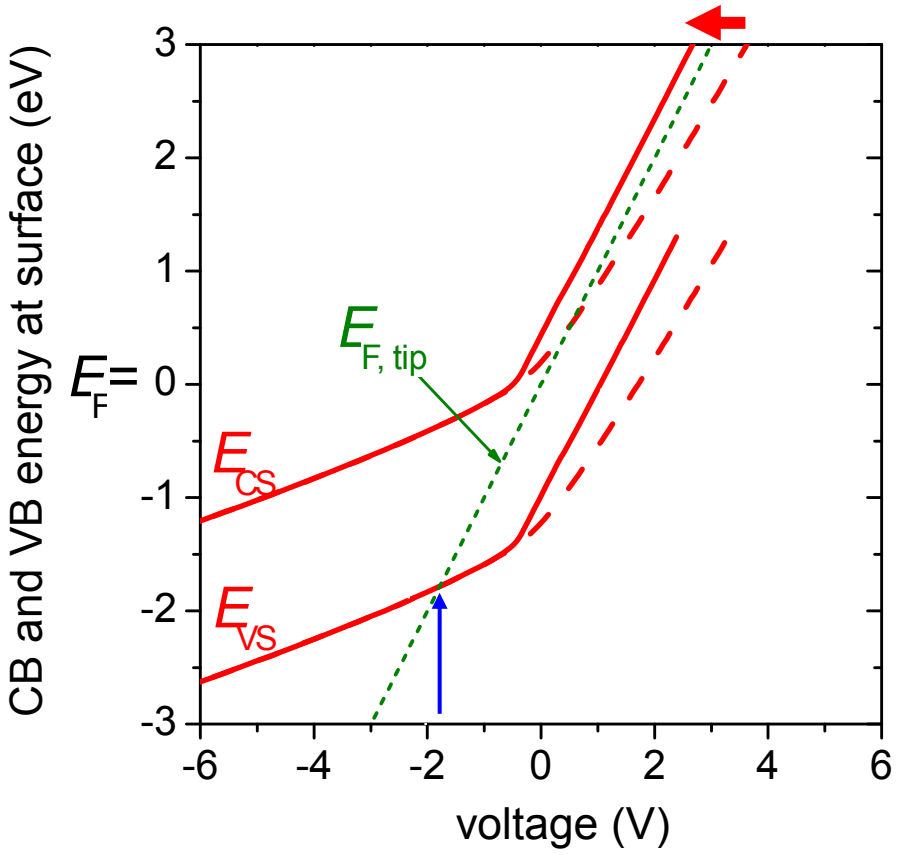
Tip-induced band bending: unpinned *n*-GaAs



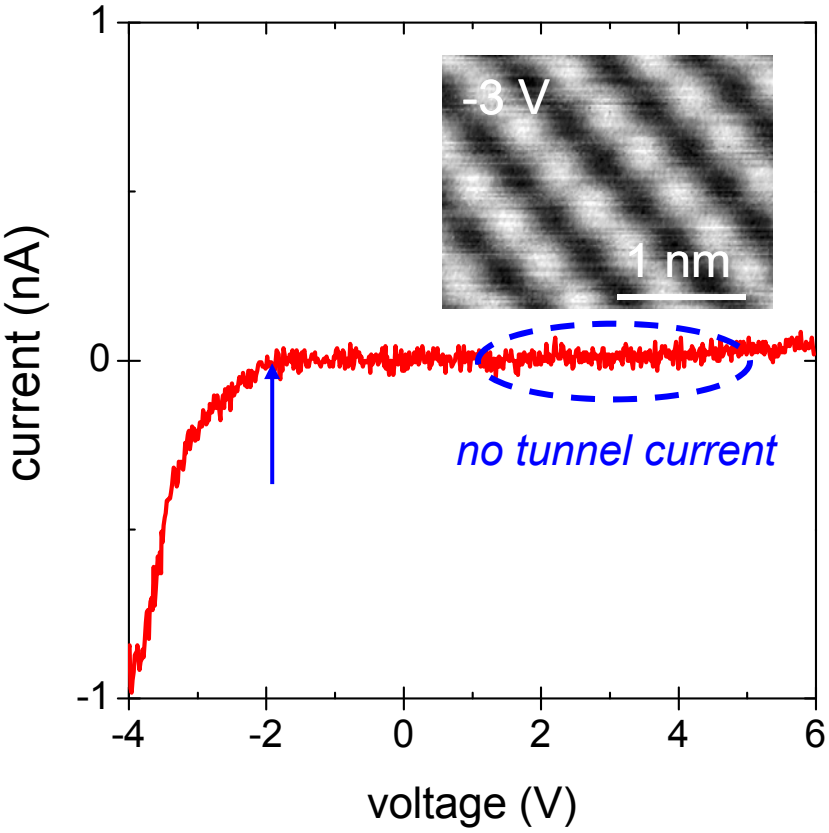


Jäger *et al.*, PRB **67**, 165327 (2003)

Semi-insulating GaAs(110): unpinned

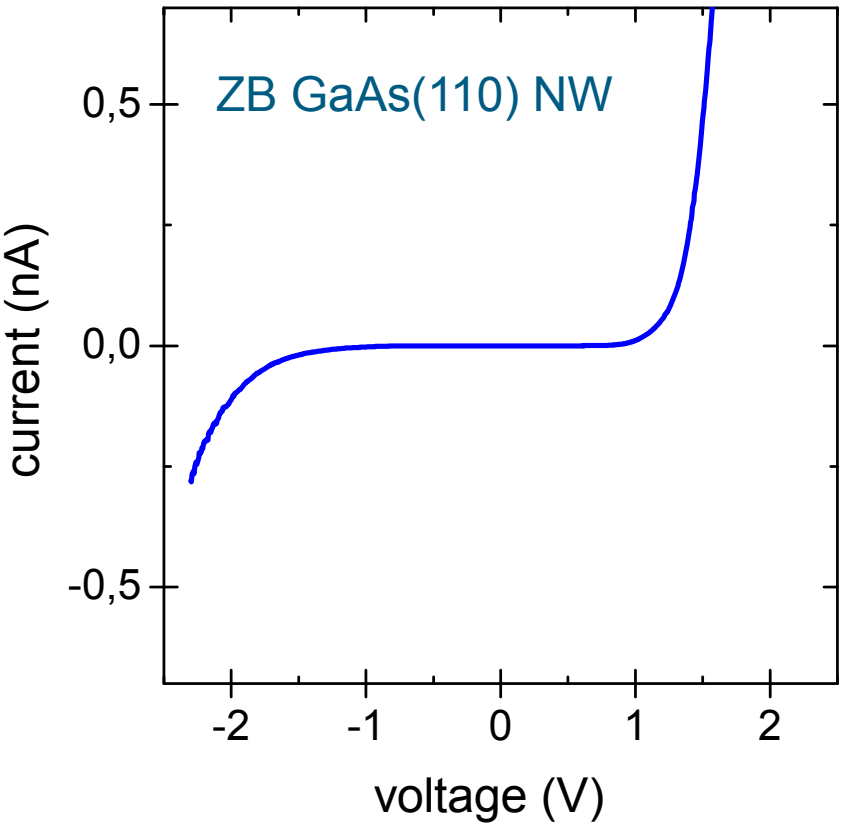


Jäger *et al.*, PRB **67**, 165327 (2003)

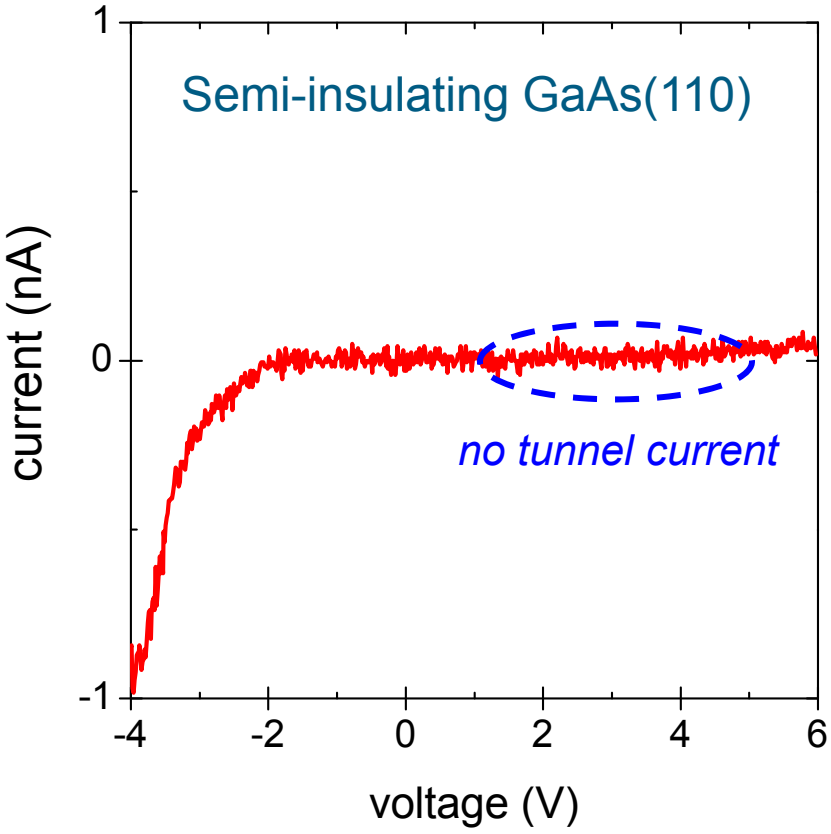


Jäger *et al.*, PRB **65**, 195318 (2002)

Undoped NW vs. SI-GaAs

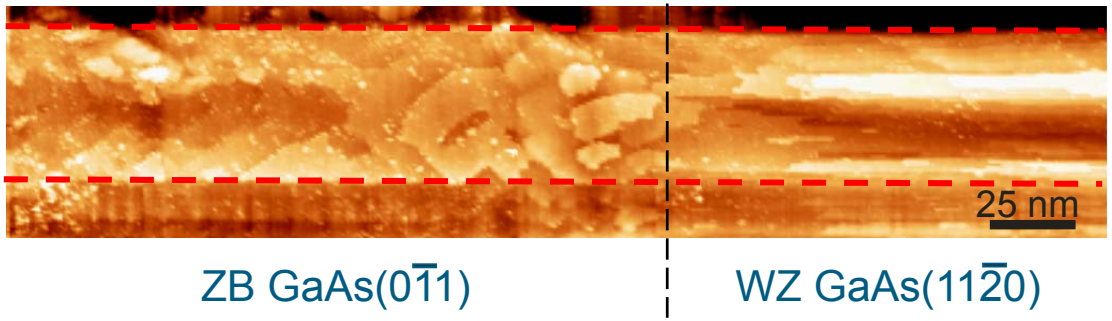


Capiod *et al.*, APL **103**, 122104 (2013)



Jäger *et al.*, PRB **65**, 195318 (2002)

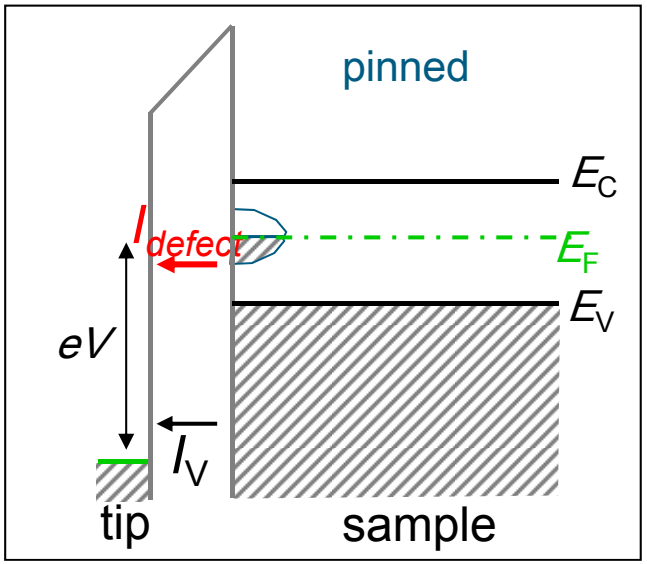
Pinning by surface steps



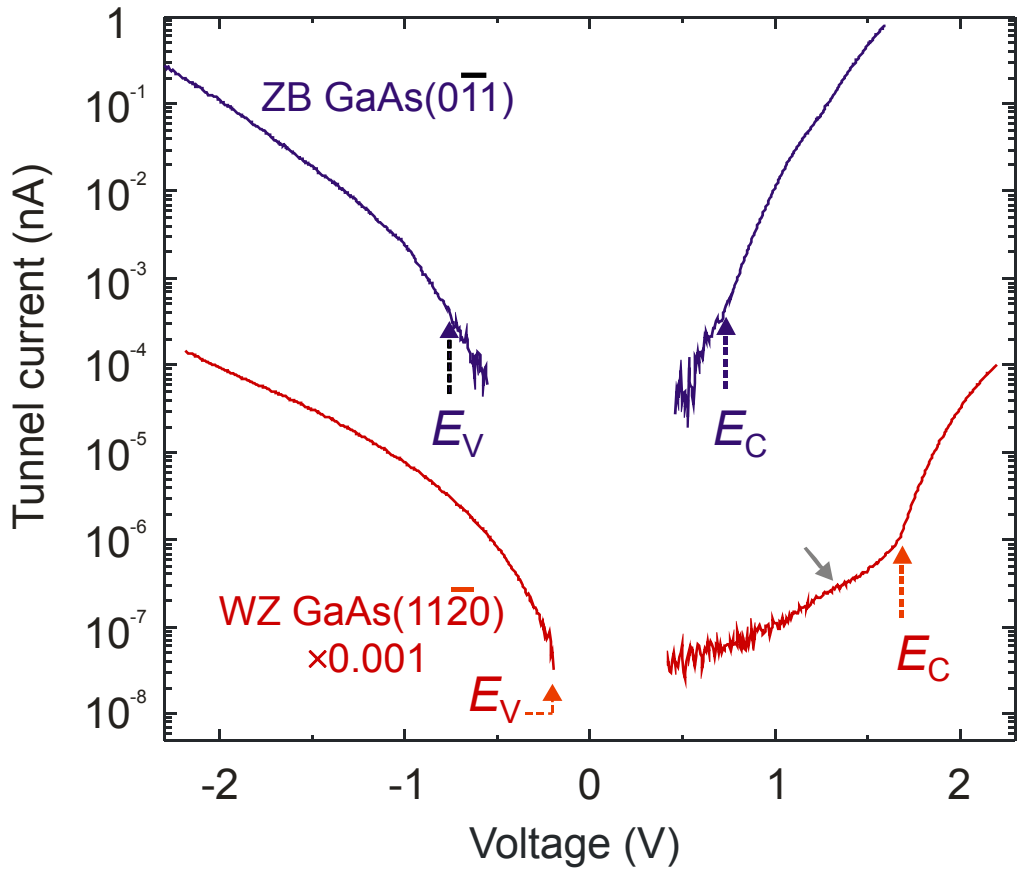
Step density: 10^5 cm^{-1}

$\triangleq$

defect state concentration: 4×10^{13} cm^{-2}



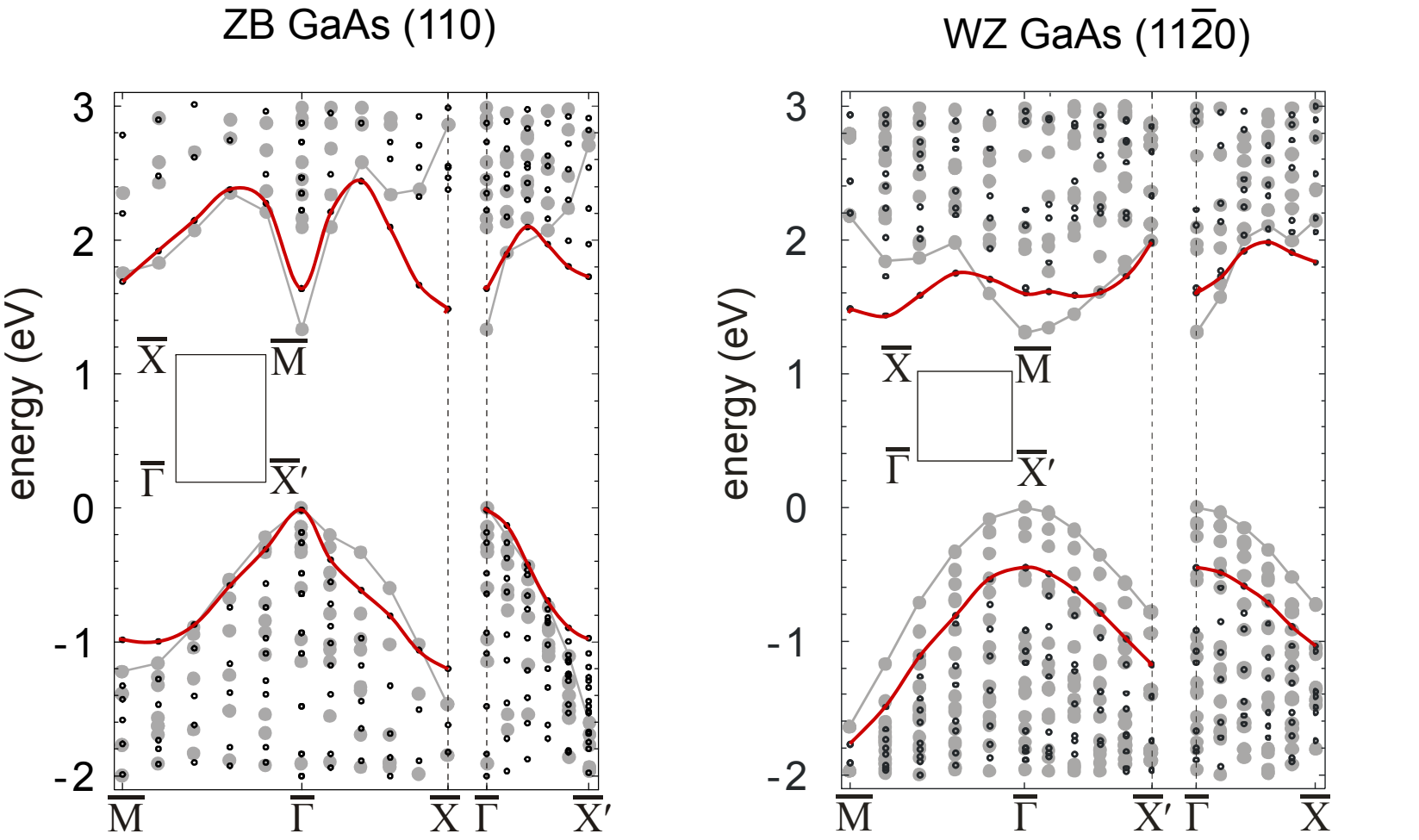
Scanning tunneling spectroscopy: ZB and WZ sections



Capiod *et al.*,
APL **103**, 122104 (2013)

→ Real band gaps not deformed by electric field

Calculated surface band structure

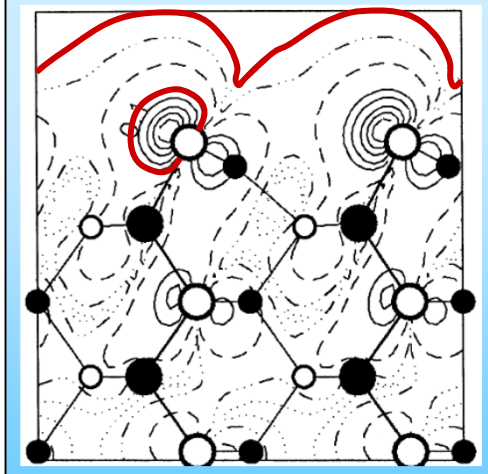


Capiod et al., APL **103**, 122104 (2013)

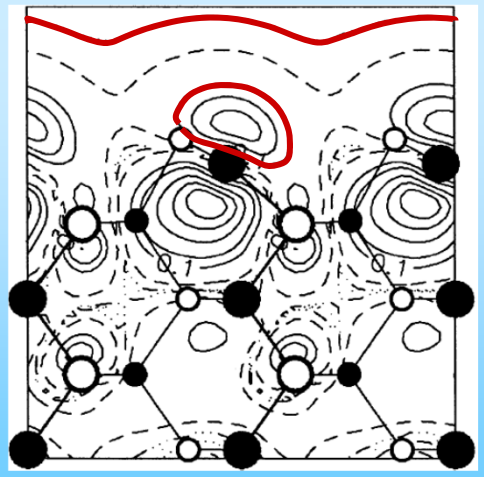
Measured vs. calculated band gaps

Facet	Experimental	Theory	
		Bulk band gap	Surface band gap
ZB GaAs {110}	1.5 eV	1.33 eV	1.50 eV
WZ GaAs {11$\bar{2}$0}	1.9 eV	1.30 eV	1.88 eV

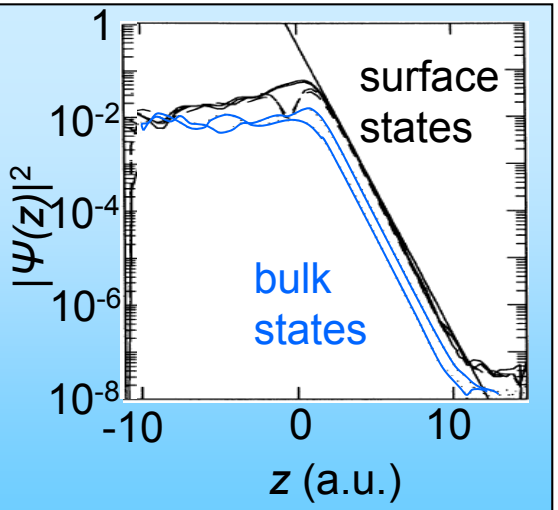
Capiod et al., APL **103**, 122104 (2013)



Filled A_5 state



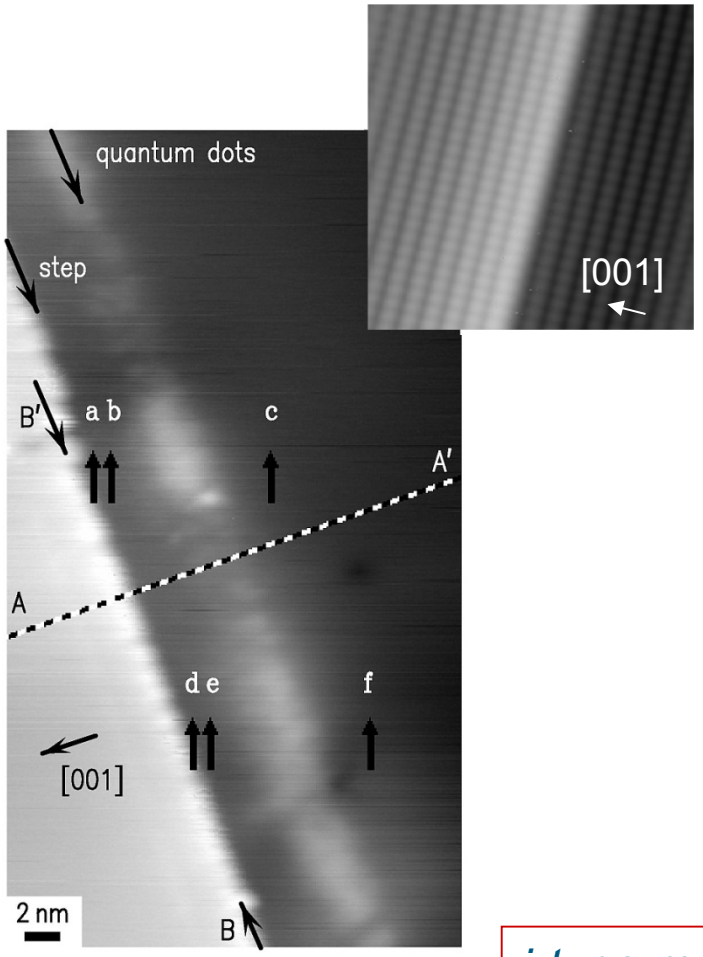
Empty C_3 state

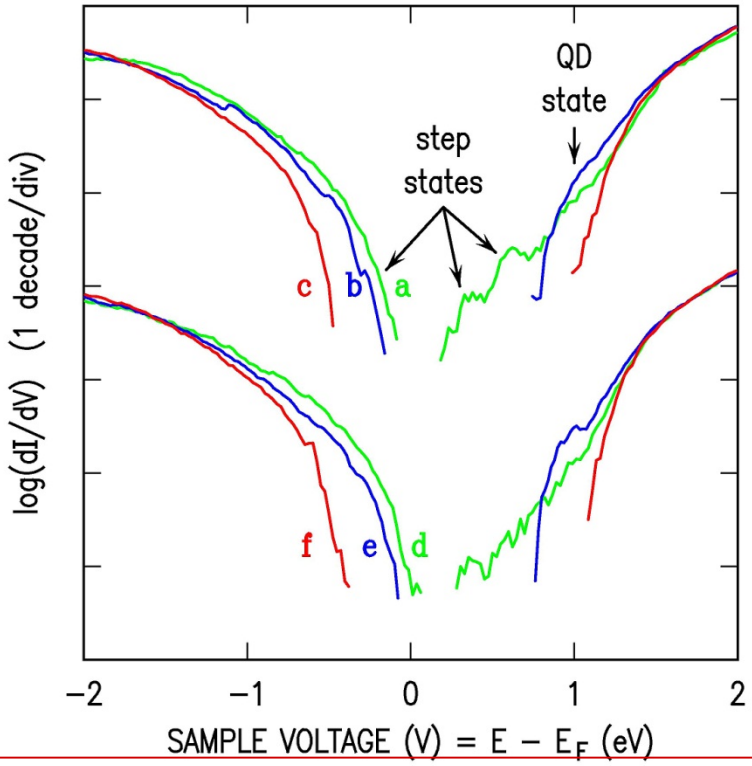


Engels *et al.*, PRB **58**, 7799 (1998)

→ STS probes *surface* band gaps and *surface* band egdes !

Defect states: Steps on undoped GaAs(110)

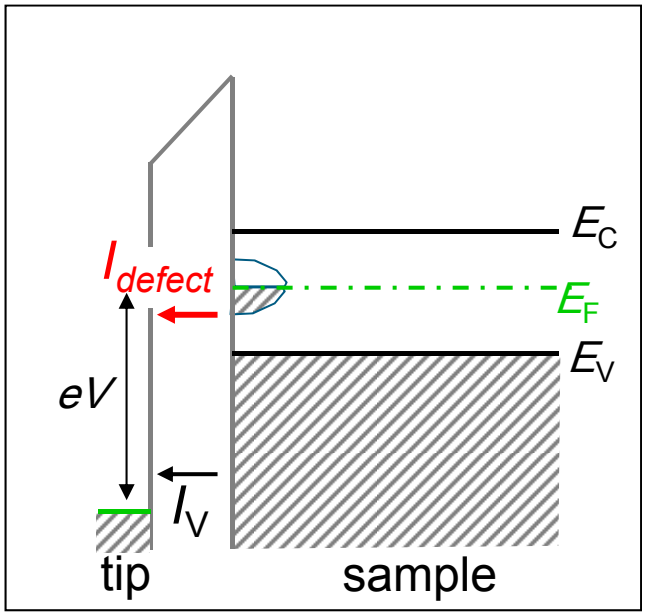




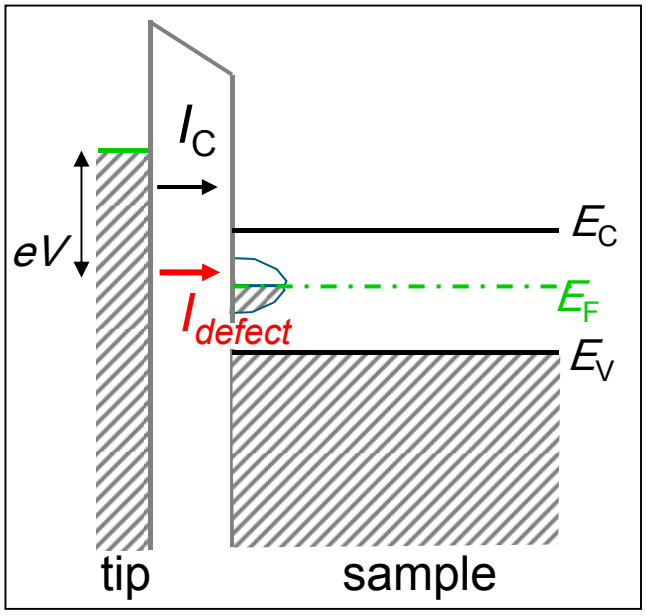
S. Gaan *et al.*,
Surf. Sci., **606**, 28 (2012).

i-type materials:
Step states induce a tunnel current within the gap near valence and conduction band edges

Mid-gap defect states induced by steps

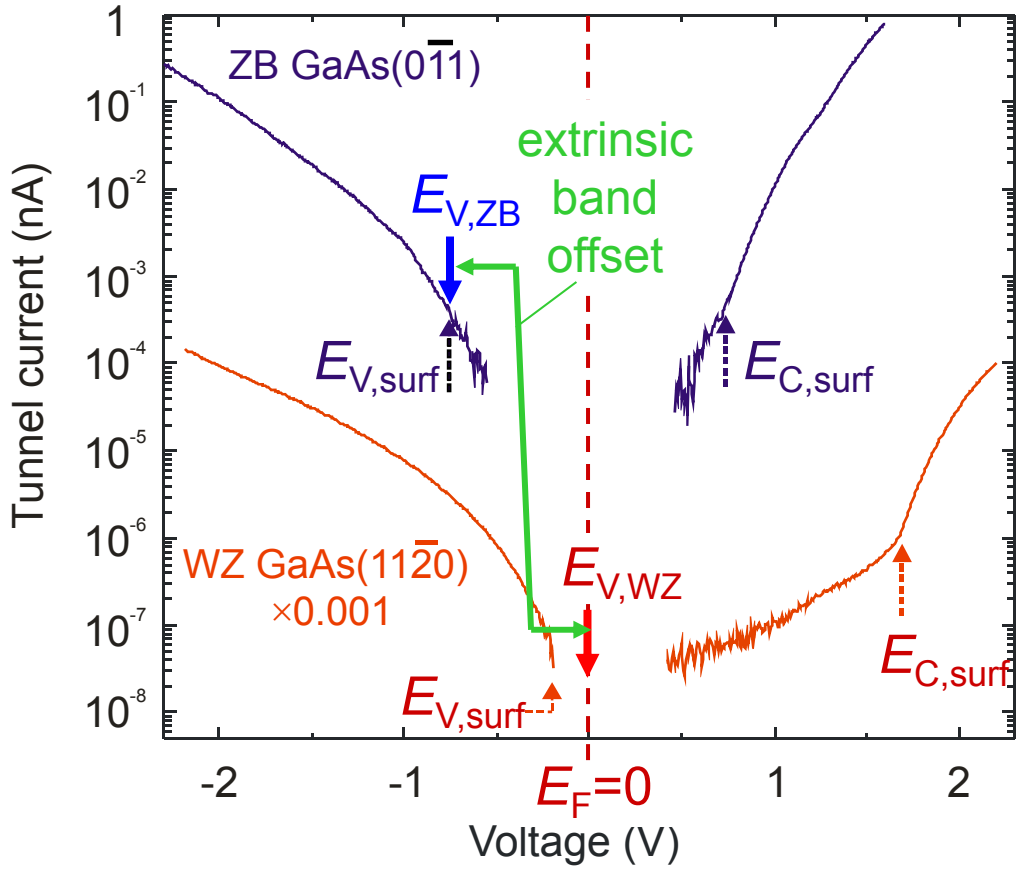


negative voltages



positive voltages

p-i junction on NW surfaces at WZ-ZB interface

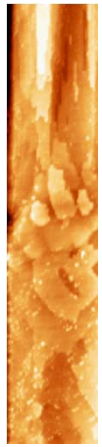


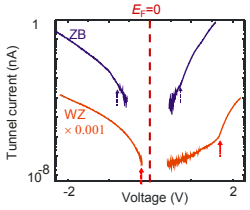
→ $E_{F,Zincblende} = (E_{V,ZB}+0.7) \pm 0.1$ eV
$E_{F,Wurtzite} = E_{V,WZ} \pm 0.2$ eV

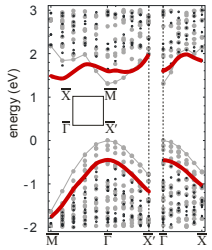
→ $p_{Wurtzite}$ - $i_{Zincblende}$ junction

Capiod *et al.*, APL **103**, 122104 (2013)

Conclusions







STM and STS on GaAs WZ-ZB NWs: probes *surface band edges*; fully *pinned sidewall* surfaces

Different Fermi level pinning at the ZB and WZ surface

Extrinsic band offsets of ~0.7 eV at the WZ-ZB interface in the near surface region of the NW creating *p-i junction*.

Extrinsic band offset screened toward the NW center

Large sidewall pinning-induced extrinsic offsets likely affect carrier transport to a greater extent than the very small bulk GaAs offsets at WZ-ZB interfaces.

Acknowledgment

- P. Capiod, T. Xu, J. P. Nys, M. Berthe, P. Caroff, B. Grandidier *(Lille)*
- G. Patriarche *(Marcoussis)*
- L. Lymperakis, J. Neugebauer *(MPIE Düsseldorf)*
- M. Schnedler, R. E. Dunin-Borkowski *(Jülich)*