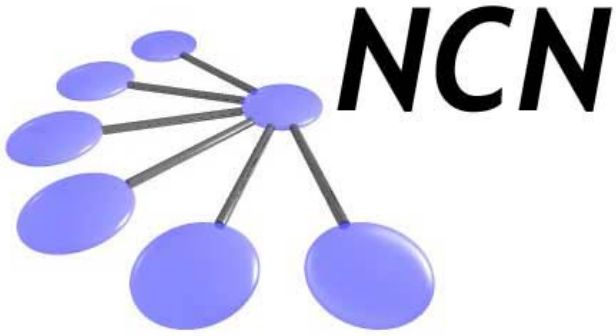
Alloy Disorder in Nanowires



PURDUE
UNIVERSITY

Gerhard Klimeck
Neerav Kharche, Timothy B. Boykin*,
Mathieu Luisier, Neophytos Neophytou,

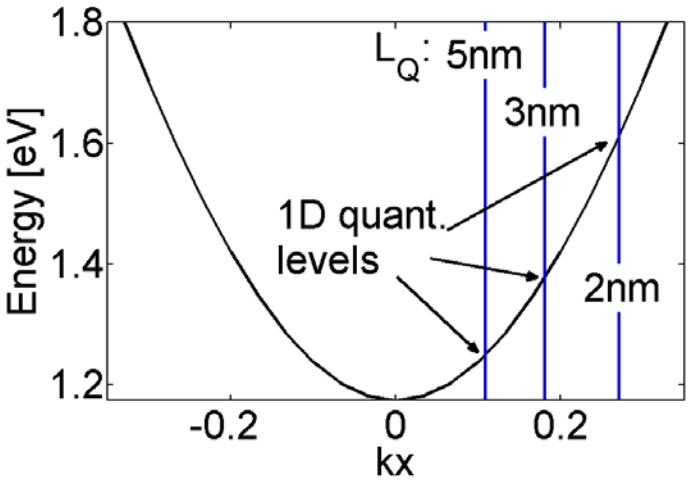
Purdue University

The effect of quantization

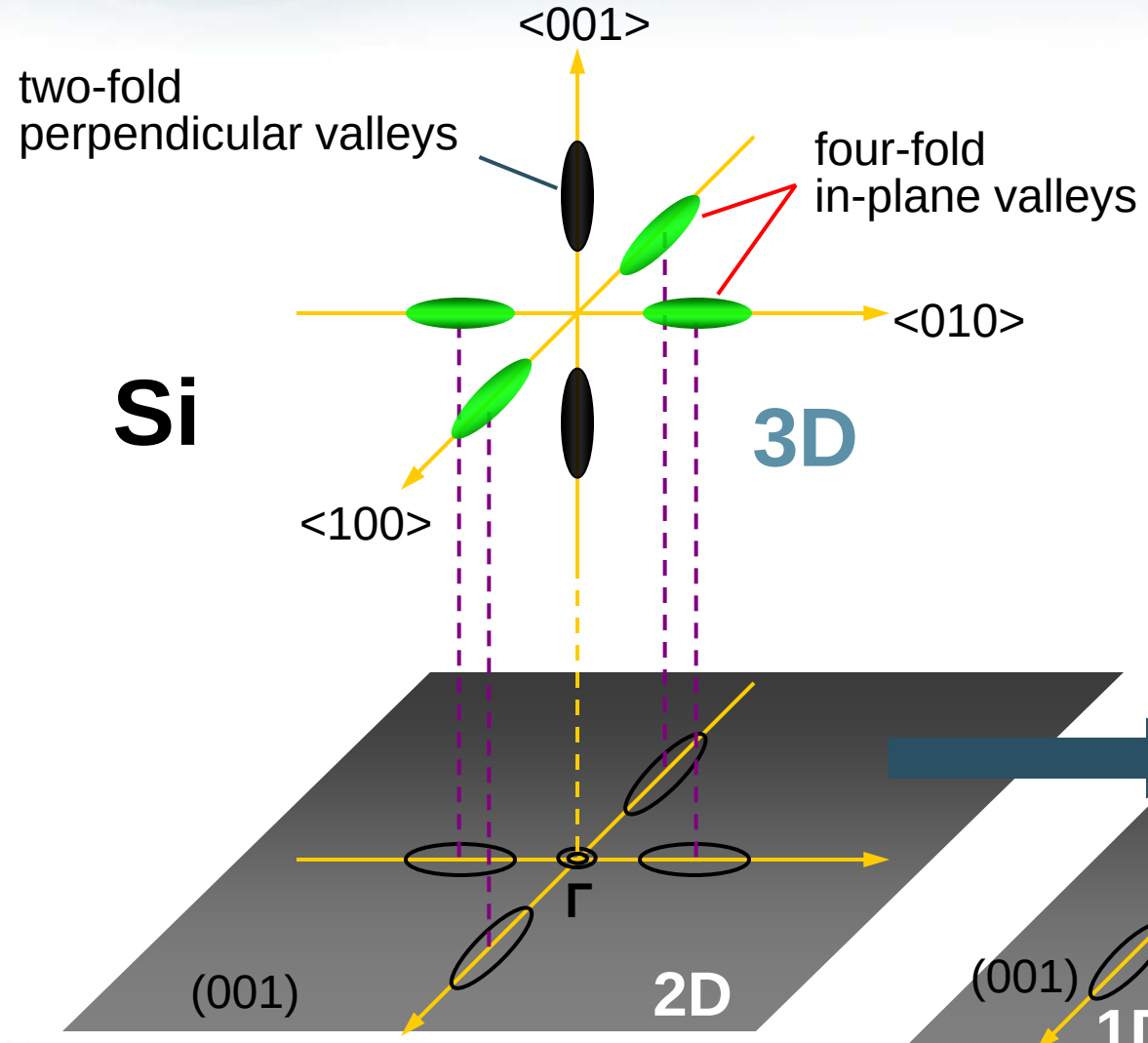
$$E_n = \frac{\hbar^2 \pi^2}{2 m_i L^2} \quad \text{(2D-quantization)}$$

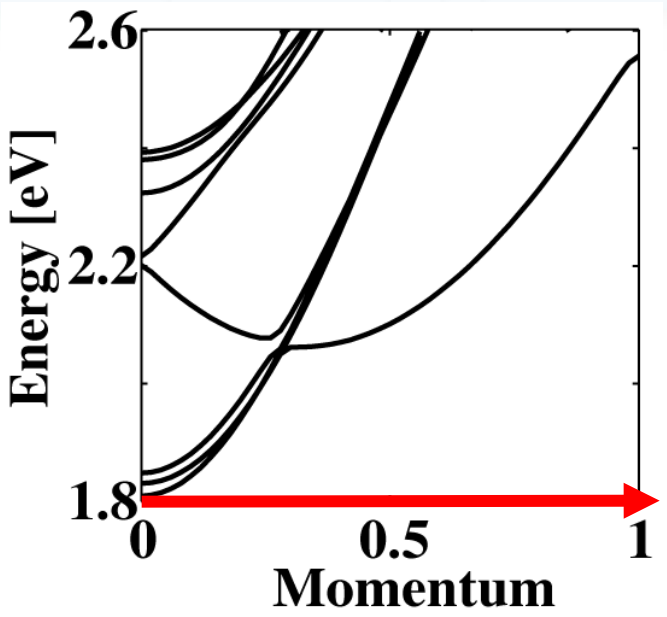
$$E = \frac{\hbar^2 k^2}{2 m_i} \quad \text{(parabolic mass)}$$

$$\rightarrow \; k = \frac{\pi}{L}$$



From 3D to 1D E(k) contours

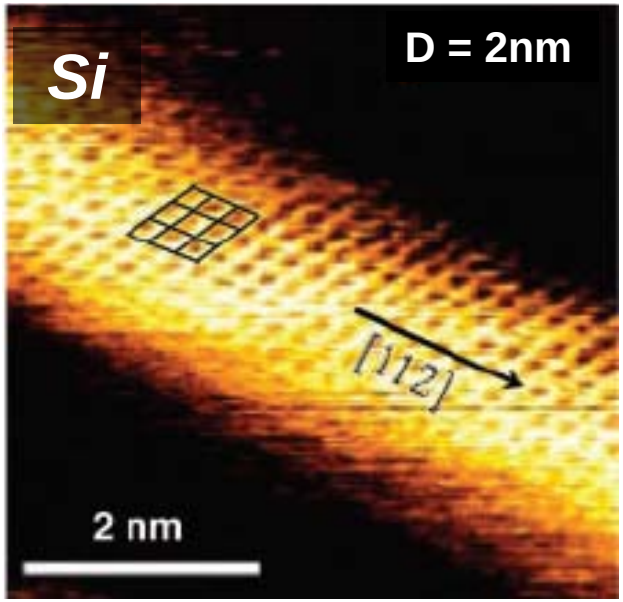




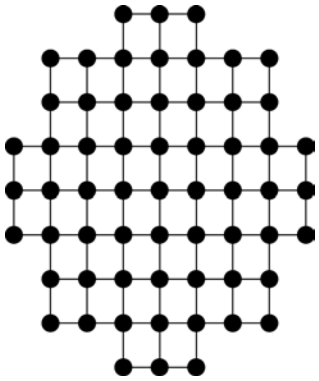
Projection to 1D

4 X equivalent valleys at **Γ**

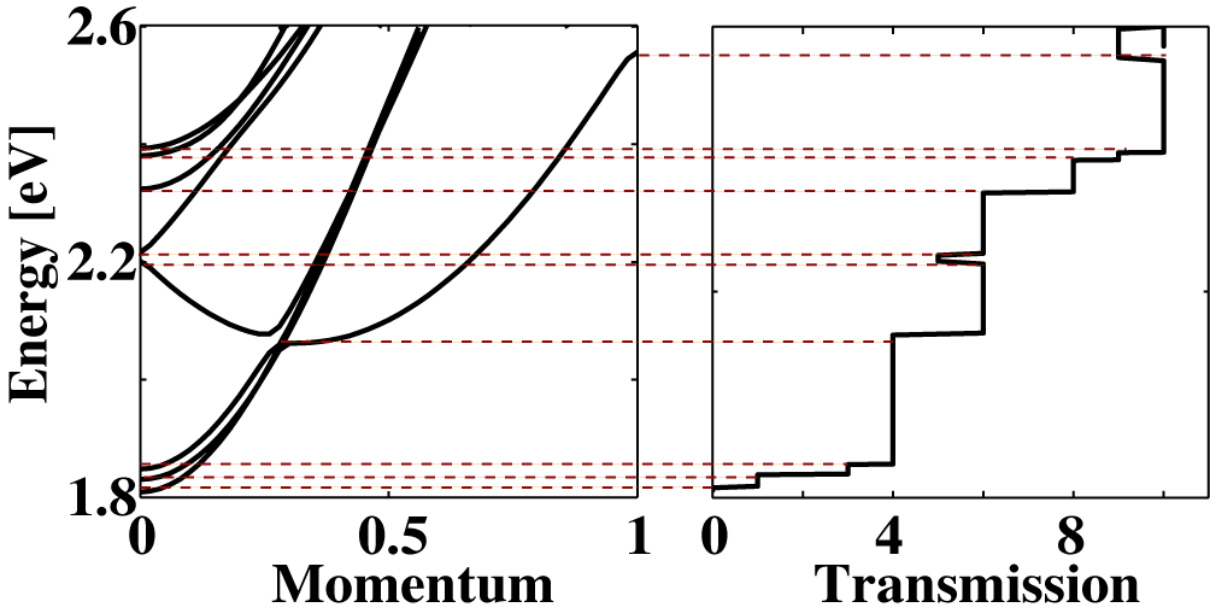
"Perfect" Nanowires



Ma et al., Science, 299, 1847, 2003

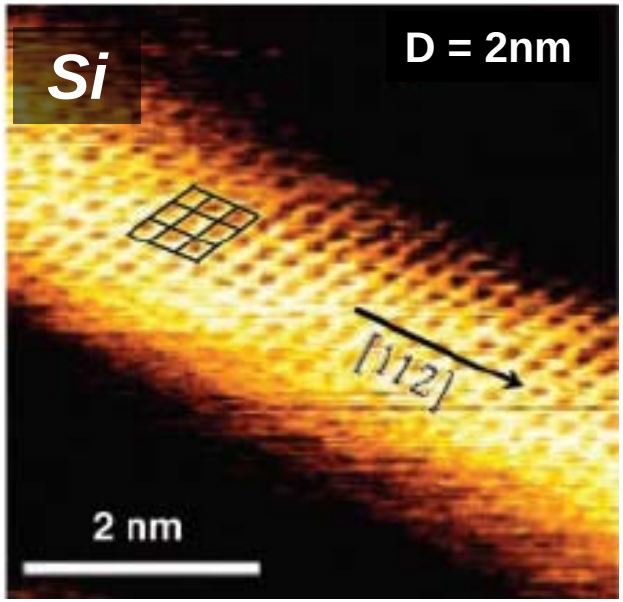


Simulated:
2nm [001] wire
infinitely long

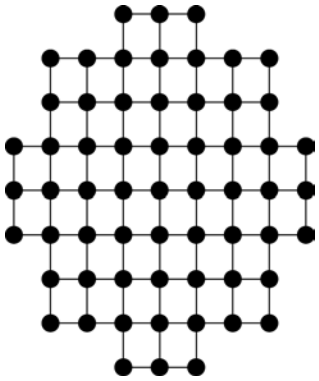


- Every band => transmission channel
- Transmission is quantized

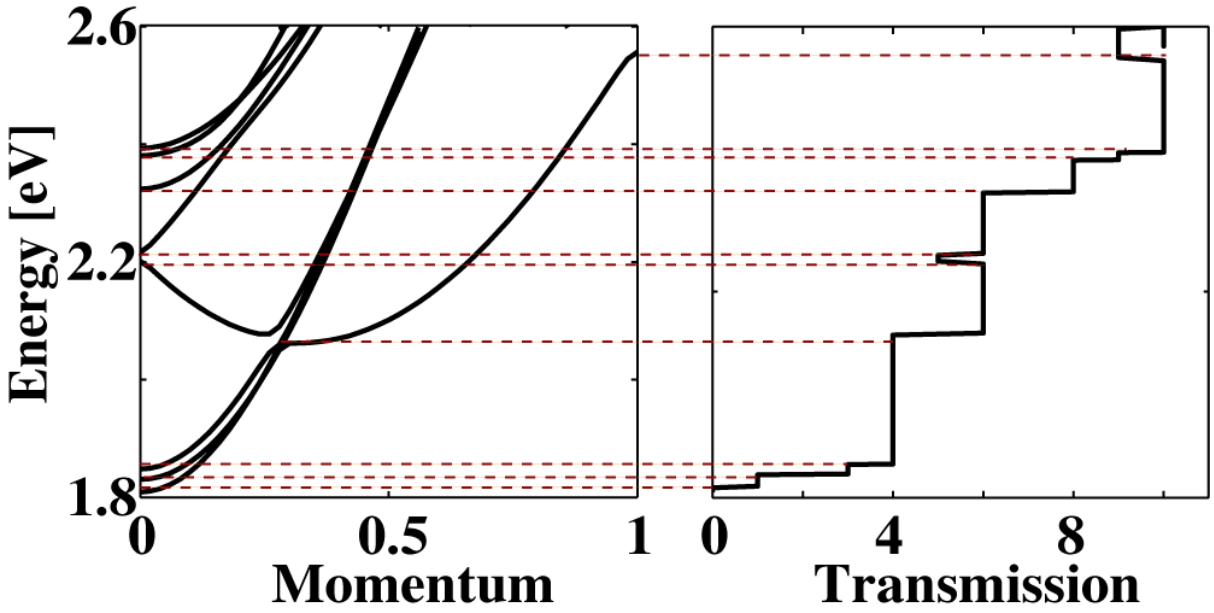
"Perfect" Nanowires



Ma et al., Science, 299, 1847, 2003

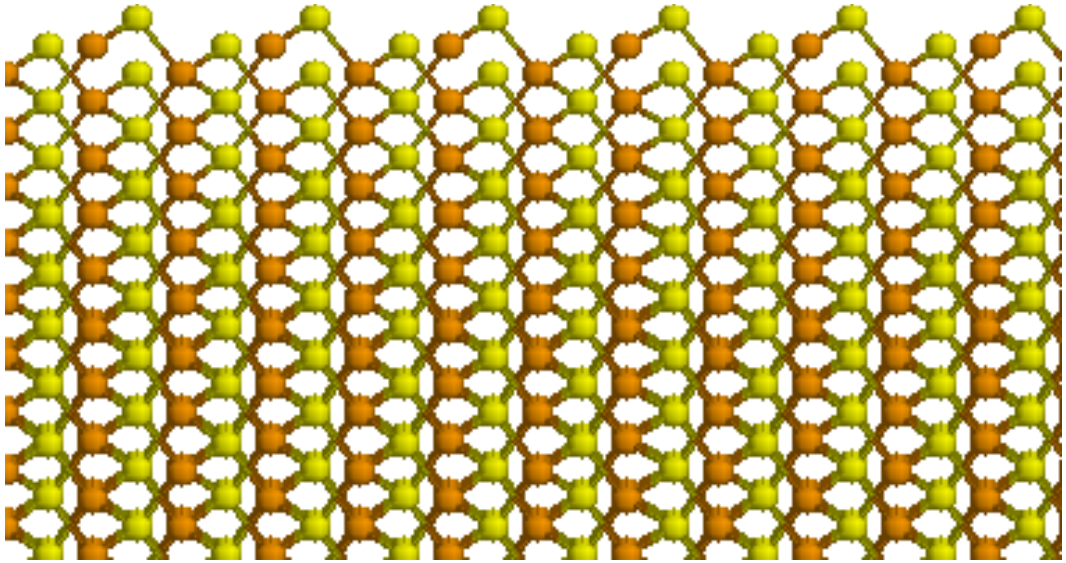


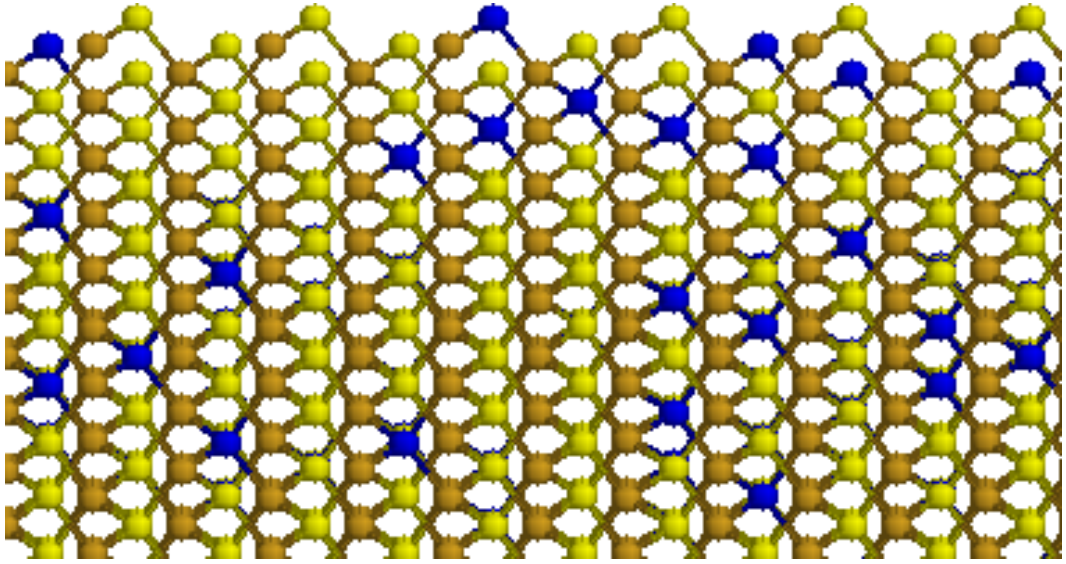
Simulated:
2nm [001] wire
infinitely long



- Every band => transmission channel
- Transmission is quantized

AlGaAs alloy nanowire
Adding Al into GaAs



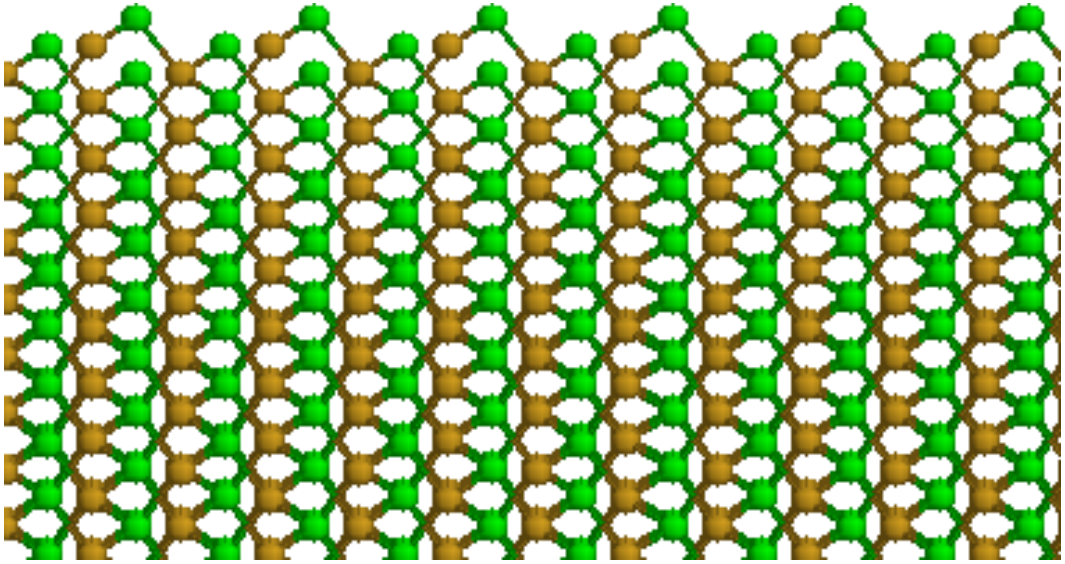


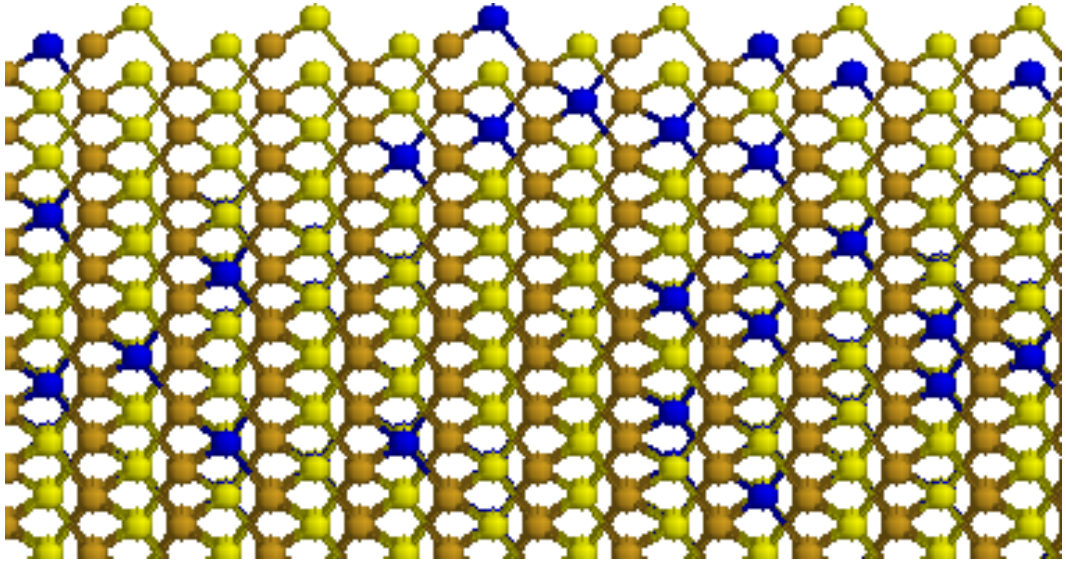
Ordered nanowire
-perfect GaAs

Insert
Al

Alloyed nanowire
-locally disordered
-Not periodic

AlGaAs alloy nanowire
VCA Average



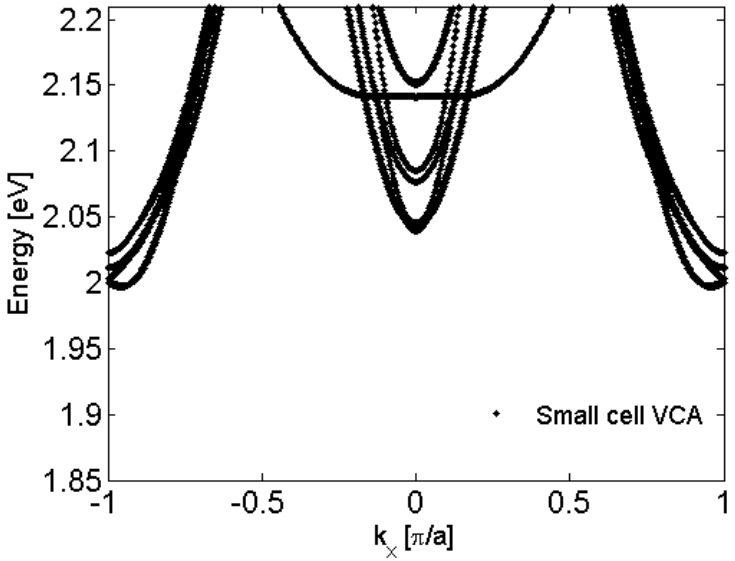


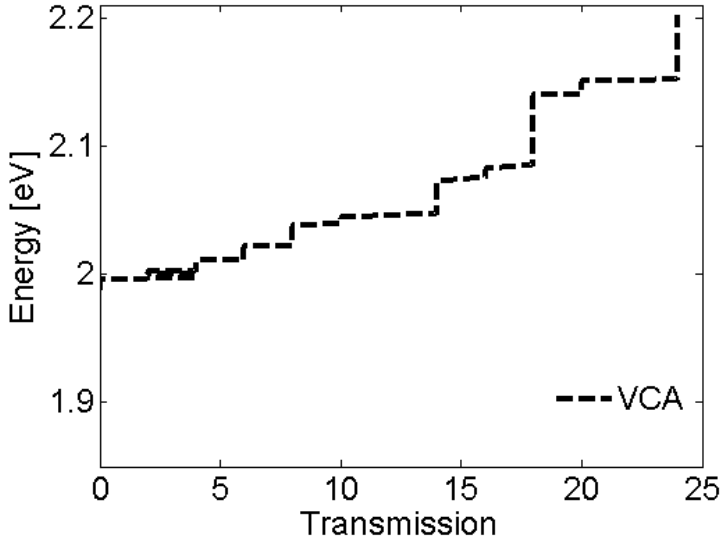
Alloyed nanowire
-Average Al and Ga
-locally ordered
-Periodic

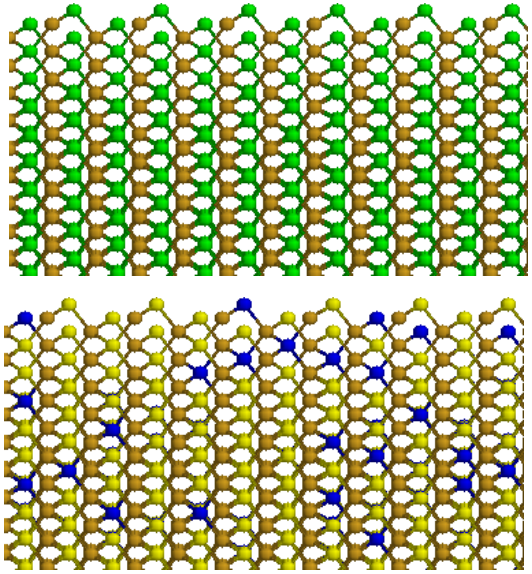
Typical Approach: VCA

Alloyed nanowire
-locally disordered
-Not periodic

Bandstructure and transmission of VCA AlGaAs alloy nanowire





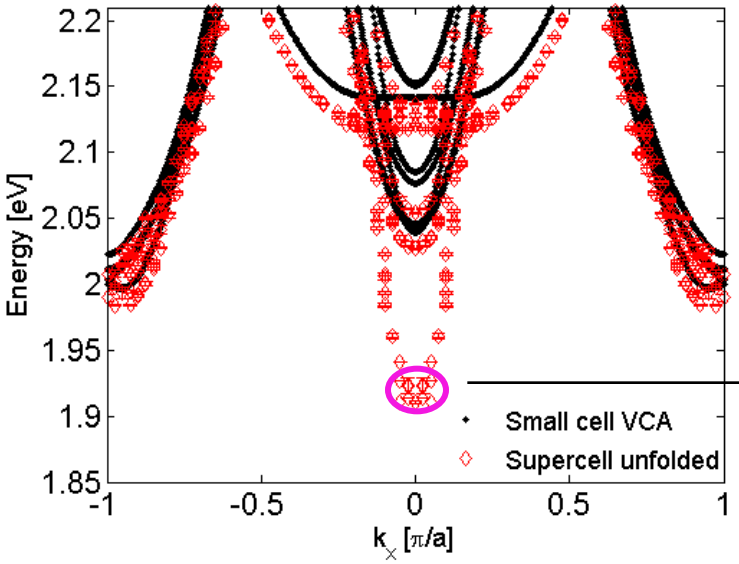


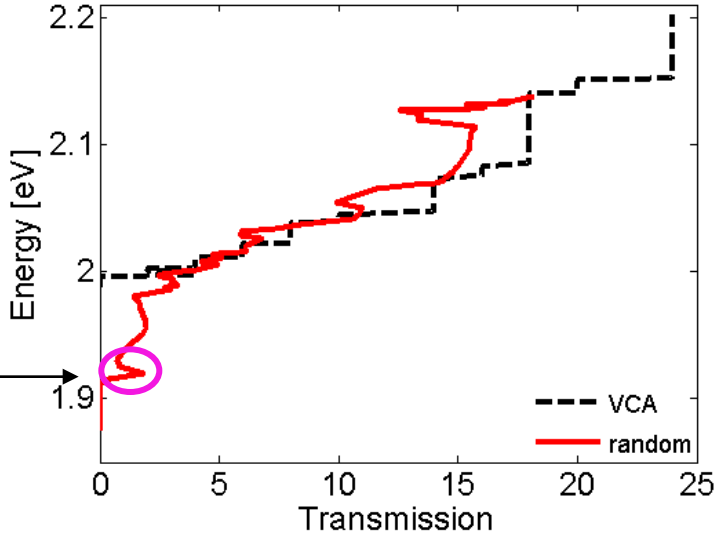
?

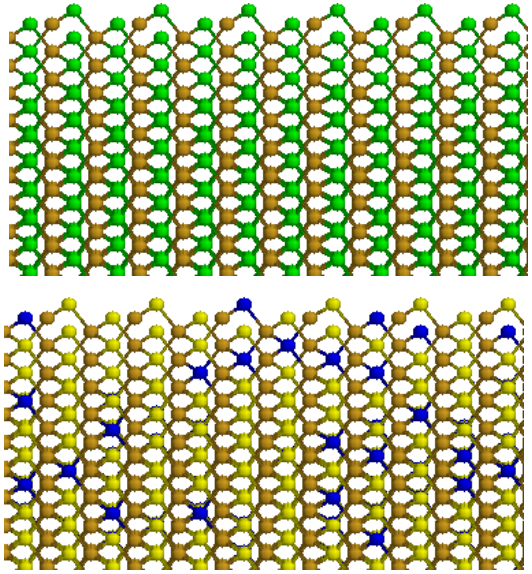
VCA Alloyed nanowire
-Average over Al and Ga
-locally ordered
-periodic
-every band has step transmission

Truly Alloyed nanowire
-locally disordered
-Not periodic

Bandstructure and transmission of VCA AlGaAs alloy nanowire



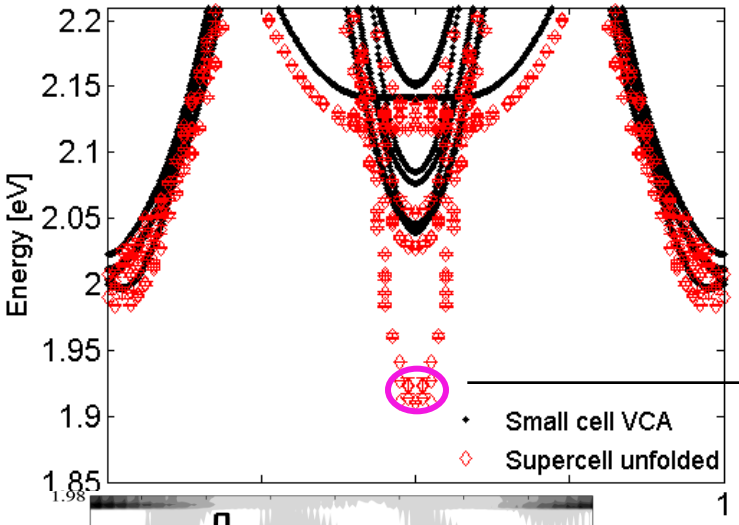


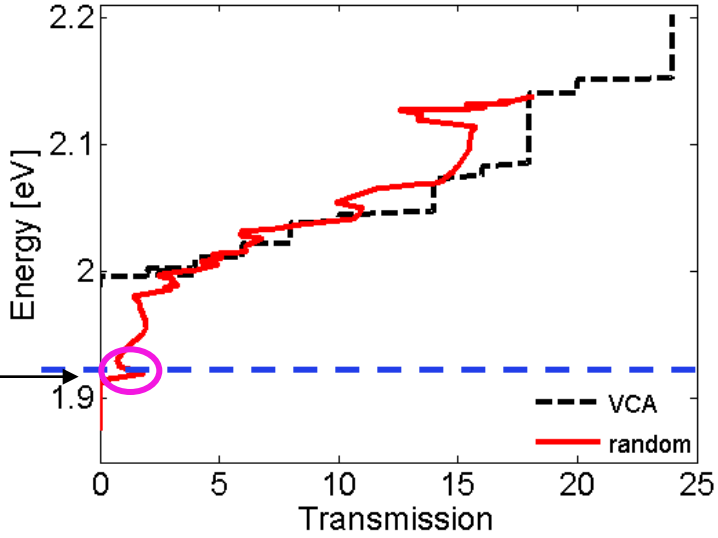


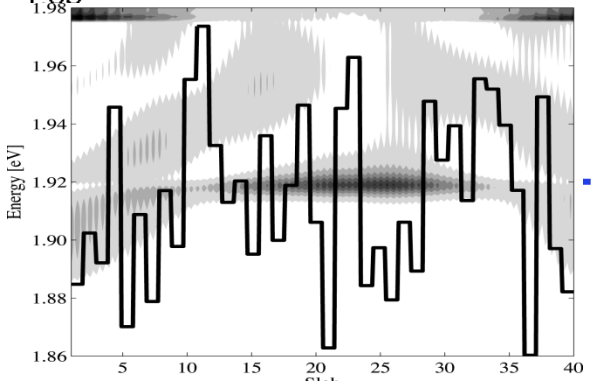
VCA Alloyed nanowire
-Average over Al and Ga
-locally ordered
-periodic
-every band has step transmission

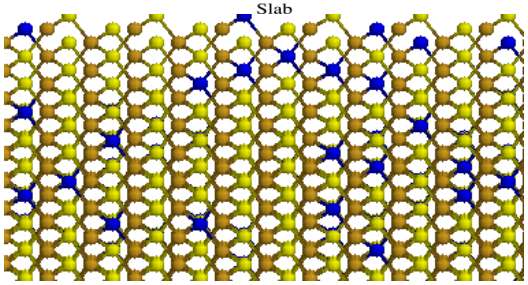
Truly Alloyed nanowire
-locally disordered
-Not periodic
-Approximate bandstructure - lower bandgap
-Transmission - no steps - resonance features

Bandstructure and transmission of VCA AlGaAs alloy nanowire





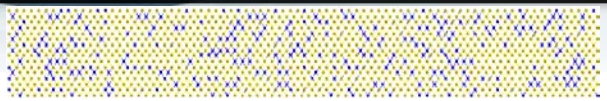


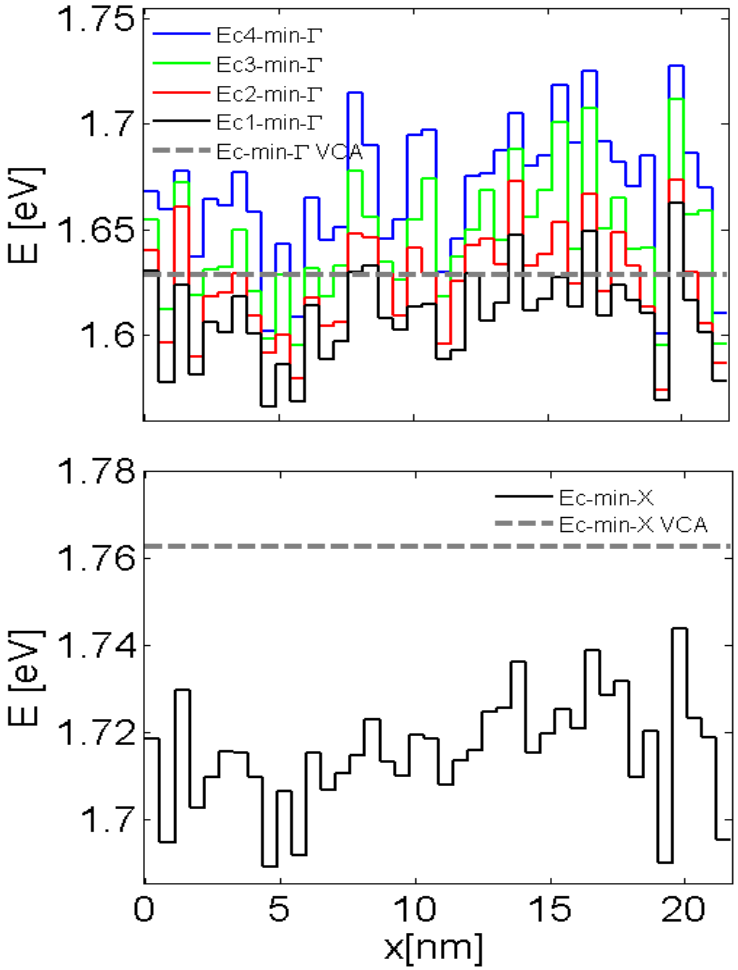


VCA Alloyed nanowire
-Average over Al and Ga
-locally ordered
-periodic
-every band has step transmission

Truly Alloyed nanowire
-locally disordered
-Not periodic
-Approximate bandstructure - lower bandgap
-Transmission - no steps - resonance features
-Localized states - resonant tunneling

SiGe nanowire

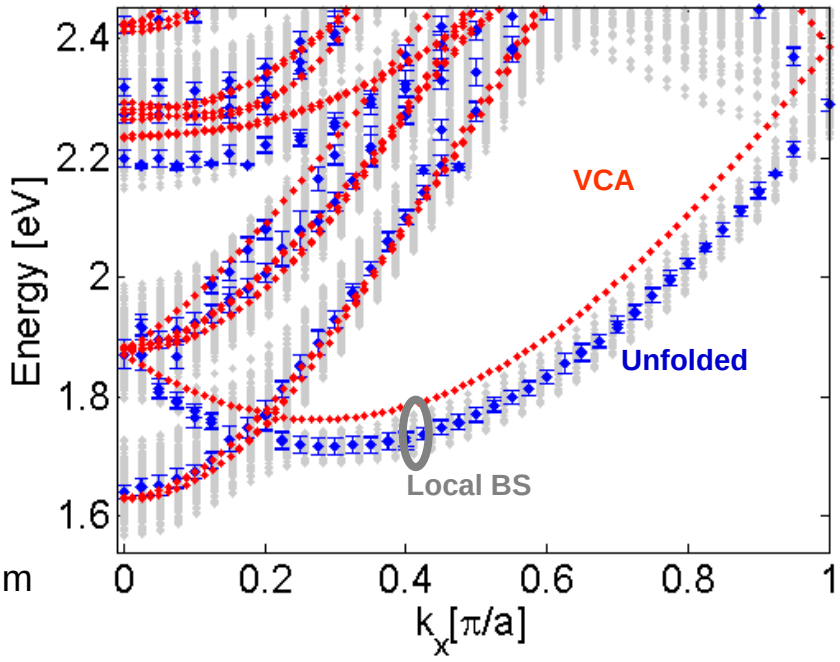




Bandedge minima first four conduction subbands (Δ_4 valleys)

Bandedge minimum transport direction (Δ_2 valleys)

VCA is not a good approximation for Δ_2 valleys



Special Issue on Nanoelectronic Device Modeling in *IEEE Transactions on Electron Devices* (2007)

Conclusions on Alloy Disorder in Nanowires

- Alloy wires are NOT smooth
- “Conduction band edge” flucatuates locally
- Dispersion changes
- Transmission and Density of states show localization effects