Why SiGe material?

**MOTIVATION**

- Higher drive current and shrinking device dimensions - Moore’s Law
- New channel material for higher current

**OBJECTIVE**

- Development of Electronic Structure model for SiGe
  - Virtual Crystal Approximation (VCA)
  - Random Alloy Treatment (RAT)
- Understand alloy disorder in SiGe for transport
- Extract mobility information using Green’s Function approach

Electronic Structure: VCA method

- Tight binding based Virtual Crystal Approximation (TB-VCA)
- Critical design parameters are well reproduced by VCA

Bulk SiGe electronic properties captured well by TB-VCA

Transport in Core/Shell SiGeSi – TB VCA

- Spatial distribution of current in SiGe core-shell wires
- On-state current distribution in SiGe core-shell p-n FET

VCA provides captures spatial trends but misses randomness

Random Alloy Treatment (RAT)

- SiGe - alloy with inherent disorder
- No periodicity or concept of E$k$($k$)
- Treat Si and Ge atoms separately

Relax SiGe structure using VFP Keaning model:
- Parking test - Bonds maintain distinct bulk values

SiGe bond length benchmarking

- Random Alloy Treatment (microscopic)
- SiGe scattered potentials from RAT

Bulk SiGe bandedges using supercell

- Random Alloy Treatment (microscopic)
- SiGe composable for bandedge calculation

SiGe scattering parameter not a ‘constant’ with composition

Transport in Alloy: Green’s Function

- How to capture randomness in disordered system?
- Transmission T([I]) calculation using Green’s function provides a good way to capture disorder

Green’s function and Landauer approach can capture randomness

Comparison of Transmission

- Transmission from Green’s Function
- Transmission to terminal characteristics

Transmission terminal characteristics

- Disorder results in higher charge but reduced mobility in 1D channel

Conclusion and Future Work

- Implement VCA (VCA) homogenous material transport disorder as a perturbation
- Random Alloy Treatment represents disorder explicitly
- Transport in disordered channel using Green’s function

**FUTURE WORK**

- Calibration of Si-Ge electronic structure (tight binding parameters)
- Understanding transistors in nano-structured SiGe channel devices
- Transport simulation of Ultra Thin Body and Nanowire SiGe devices