Modeling of SiGe material for ultra-scaled CMOS device applications

A. Paul, S. R. Mehrotra, Z. Jiang, M. Luisier and G. Klimeck
Purdue University and NCN

Why SiGe material ?

MOTIVATION

Higher drive current and shrinking device dimensions : **Moore's Law**

Bulk Mobility (cm^2/Vs)[1]	Si	Ge
Electrons	1400	3900
Holes	450	1900

New channel material for higher current

3D nanostructure devices for better electrostatics.

Atomistic Approach needed to model Disordered System

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.

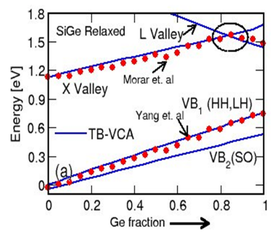
Electronic Structure : VCA method

Virtual Crystal Approximation(VCA)

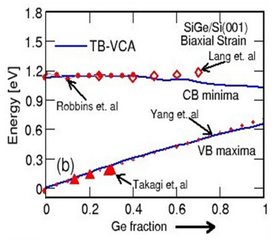
Tight-Binding based Virtual Crystal Approximation **TB-VCA**

Si + Ge → SiGe "Virtual Atom"

Results



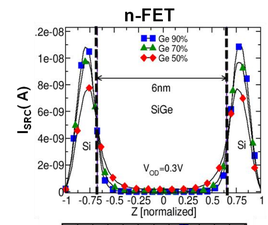
Critical design parameters are well reproduced by **VCA**[1]



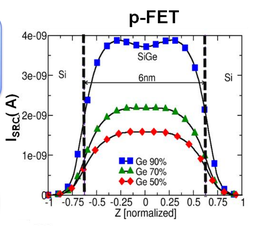
Bulk SiGe electronic properties captured well by TB-VCA.

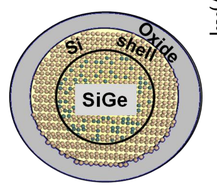
[1] A.Paul , S. Mehrotra, M.Luisier and G. Klimeck, IEEE, EDL, April, 2010

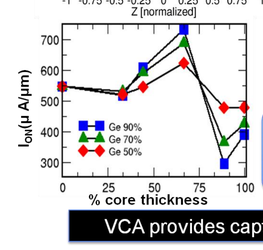
Transport in Core/Shell SiGe/Si – TB VCA



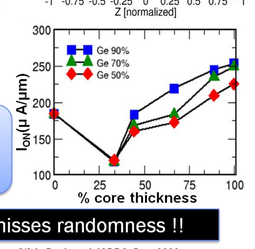
Spatial distribution of current in SiGe core-shell wires.[1]







On-state current distribution in SiGe/Si core/shell n-p FETs.[2]



VCA provides captures spatial trends but misses randomness !!

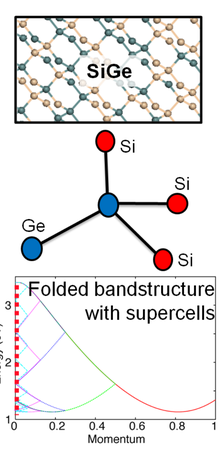
[1] A. Paul et. al, ISDRS, Dec. 2009.
[2] A.Paul et. al IEEE, EDL, April, 2010

Random Alloy Treatment (RAT)

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

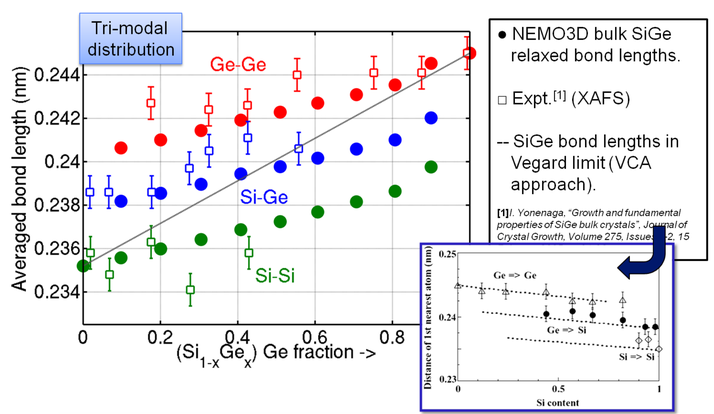
Relax SiGe structure using VFF Keating model.
Pauling limit : Bonds maintain distinct bulk value.
Vegard limit: All bonds linearly averaged .

Electronic structure using zone-unfolding[1]**.**
Supercell calculations to determine bandedges in a disordered system.



[1] Boykin at. al, PRB 71, 115215, (2005)

SiGe bond length benchmarking



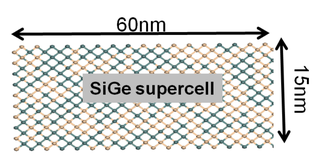
- NEMO3D bulk SiGe relaxed bond lengths.
- □ Expt.[1] (XAFS)
- -- SiGe bond lengths in Vegard limit (VCA approach).

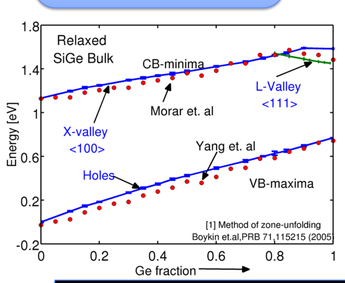
[1] *I. Yonenaga, "Growth and fundamental properties of SiGe bulk crystals", Journal of Crystal Growth, Volume 275, Issues 1-2, 15*

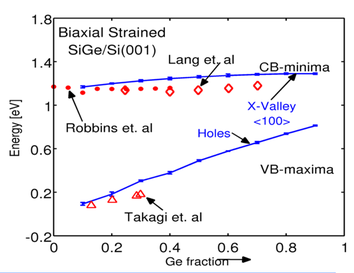
Bulk SiGe bonds are more in Pauling limit rather than Vegard limit.

Bulk SiGe bandedges using supercell

Random Alloy Treatment (microscopic) of SiGe supercell for bandedge calculation.







RAT provides good match with experimental data [1].

[1] A.Paul , S. Mehrotra, M.Luisier and G. Klimeck, IEEE, EDL, April, 2010

Alloy Scattering

CLASSICAL APPROACH

$$\mu_A = \frac{\sqrt{2\pi}e\hbar^4 N_0}{3x(1-x)m^{*5/2}} \frac{1}{(\Delta E)^2\sqrt{KT}},$$

Brook's formula[1] for alloy scattering.

Alloy Scattering with a fitting parameter →ΔE

ΔE fitted for bulk only, can change in nanostructures !

MICROSCOPIC TREATMENT
RANDOM ALLOY APPROACH

Alloy scattering potentials embedded in atomistic representation !

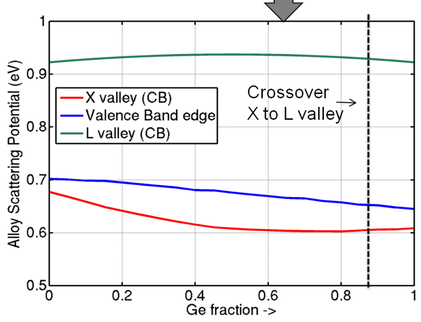
$$\Delta E^2 = \frac{N_{atom}}{x(1-x)} \overline{\langle \varphi(k_f)|H_{RAT} - H_{VCA}|\varphi(k_i)\rangle}^2$$

Random alloy provides a direct approach to treat alloy scattering.

[1] S. Krishnamurthy, et. al, APL,47, 160, (1985).

Alloy Scattering Potentials from RAT

Extracted Alloy scattering potentials (ΔE) from SiGe tight-binding theory



Band edge	ΔE (TB)	ΔE (fit used)
X valley	0.68 eV	0.7[1],0.8[2] eV
L valley	0.9 eV	0.6[3],1.0[3] eV
V.B.	~0.67 eV	0.8-1.0[3] eV 0.8141[4] eV

[1] Singh (APL 64,2985)
[2] Sturm (APL 63,2795)
[3] Fischetti (1996)
[4] Joyce (DFT) (2007)

Alloy scattering parameter(ΔE) not a 'constant' with composition !!!

Transport in Alloy: Green's Function

How to capture randomness in disordered system ?

Transmission T(E) calculation using Green's function provides a good way to capture disorder.

Transmission T(E) and Density of states g(E)

$$\sigma = \frac{2q^2}{h} \cdot \int T(E)\left[\frac{\partial F_0}{\partial E}\right] dE$$

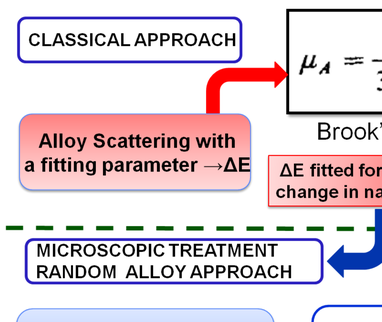
$$n = \int g(E) \cdot [F_s(E) + F_d(E)] dE$$

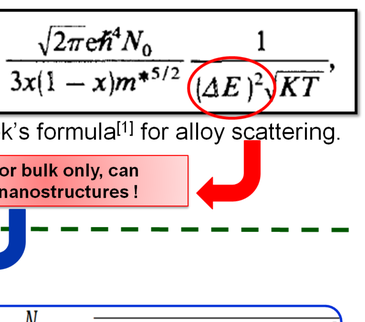
Obtain mobility $\mu = \frac{\sigma}{n.e}$

Green's function and Landauer approach can capture randomness.

Comparison of Transmission

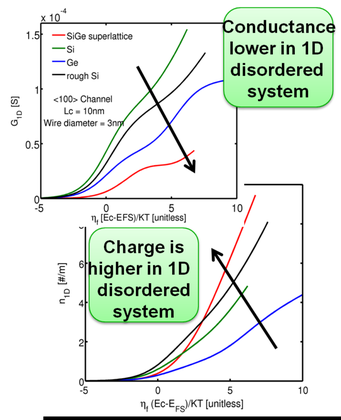
Types of devices → Transmission from Green's Function

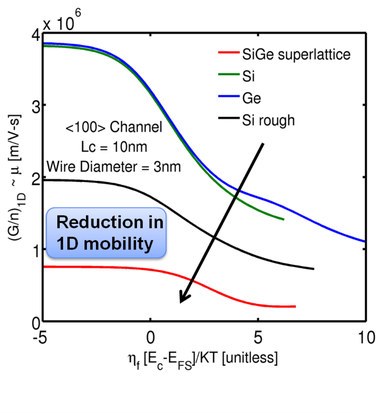




Green's function method can model disorder in the channel.

Transmission to terminal characteristics





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

Conclusion and Future Work

IMPLEMENTED METHODS

- Virtual Crystal Approximation (VCA) homogenizes material treats disorder as a perturbation.
- Random Alloy Treatment represents disorder explicitly.
- Transport in disordered channel using Green's function.

IMPACT

- Experimental data benchmarked. Perform transport in ballistic limit.
- Bond lengths and bulk alloy SiGe bandedges benchmarked.
- Benchmarked experimental alloy scattering potential(ΔE) parameter.
- Mobility computed from transmission in disordered system.

FUTURE WORK

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

2010 MSD Annual Review

NSF nanoHUB.org PURDUE UNIVERSITY