Valence Band Energy Offset and Effective Band Gap Extraction of strained-Si/strained-Ge Type-II Heterostructures on Relaxed SiGe
Motivation

- The s-Si/s-Ge has the potential for interesting applications due to the deep valence band well of s-Ge and the small effective band gap between the conduction band of s-Si and the valence band of s-Ge.

- However, both the valence band offset and effective band gap between s-Si/s-Ge is poorly known.

- This work extracts these parameters from experimental MOS-capacitors by fitting quantum mechanical simulations to experimental QSCV data.
Applications

- **Group IV Tunneling Transistor**

- **Buried Ge channel MOSFET**


Outline

- Previous Work
- Valence Band Offset Extraction Method
- Experimental and Simulated CV Curves
- Parameter Sensitivity of the CV Technique
- Extracted Values Compared to Theory
- Conclusion
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Previous Work, Device Structure
Research by Cait Ni Chleirigh

Red text indicates differences from current device structure.

Low-T oxide

\[ \text{s-Si} \quad \text{s-Si}_{1-x}\text{Ge}_x \quad \text{Si}_{1-x}\text{Ge}_{xs} \]

\[ \Delta E_v \]

\[ \Delta 2 \]

\[ \Delta 4 \quad \Delta 6 \]

\[ E_{G,\text{eff}} \]

HH & LH

Previous Work, Valence Band Offset Research by Cait Ni Chleirigh

Goal: to extract valence band offset of s-Si/s-Ge on relaxed SiGe

This Work, Device Structure

- 1 µm Al
- 10 nm WN
- 6 nm Al₂O₃ high-κ dielectric
- Tensilely strained-Si (6 nm)
- Compressively strained-Ge (6 nm)
- 40% SiGe Relaxed Buffer (1 µm)
- p- 2 to 40% SiGe Graded Buffer (4 µm)
- p+ Si substrate
- 1 µm Al

Forming gas anneal, 450°C for 30 min
Changes from Previous Work

- **Device Structure**
  - $s\text{-Si}_{1-x}\text{Ge}_x \rightarrow s\text{-Ge}$
  - Larger $x_S$ (Ge fraction in relaxed $\text{Si}_{1-x_S}\text{Ge}_x$ substrate)
  - High-κ dielectric instead of low temperature oxide

- **Simulations**
  - **Quantum Mechanics**
    - Density Gradient Model $\rightarrow$ full Schrodinger solver
  - **Strain**
    - Band edge model $\rightarrow$ full-band quantum simulator
    - Modified valence band density of states, $N_v \rightarrow 6x6$ $k\cdot p$ method that accounts for nonparabolicities in valence band

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**Valence Band Extraction Method**

QSCV can be divided into 4 regions:
- **I**: hole accumulation in the Si cap
- **II**: hole accumulation in the Ge well
- **III**: hole depletion from the Ge well
- **IV**: electron inversion in the Si cap

Width of **II** is determined by the valence band offset between s-Si/s-Ge.
Valence Band Extraction Method

Experimental Data for 40% SiGe MOS-C

![Graph showing capacitance per area vs. gate voltage for different regions I to IV.](image)
Larger the valence band offset, the larger region II

- For a larger valence band offset, more gate voltage has to be applied to bring holes into the s-Si.
- Thus, width of II is directly related to the valence band offset.

Extraction procedure

- Measure QSCV from fabricated devices.
- Fit quantum mechanical QSCV simulations to experimental data by adjusting valence band offset.
Complexities of Simulation

- Difficult Simulation Environment
  - Strain
    - Splits VB and CB of s-Si and s-Ge
    - Changes $E_G$ for s-Si and s-Ge
    - Modifies the density of states of the different bands
  - Quantum Mechanics
    - Thin layers (~ 6 nm) for the s-Si and s-Ge
    - Must properly take into account quantization effects
    - Non-uniform masses, $m_\parallel \neq m_\perp$ because of strain warps the valence band
    - Requires use of 6x6 $k\cdot p$ method
6x6 $k\cdot p$ Method,
Top Valence Band State for Ge

Energy Scale (eV)

$k\cdot p$ dispersion in the direction perpendicular to the growth direction

Valence band is NOT parabolic!

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Simulation Variables

- Dielectric (modeled as SiO\textsubscript{2})
  - Thickness

- Silicon
  - Thickness
  - Band splitting due to strain
  - Band gap
  - Band lineup compared to germanium (\(\Delta E_v\))

- Germanium
  - Thickness
  - Band splitting due to strain
  - Band gap
  - Band lineup compared to relaxed SiGe buffer

- Relaxed SiGe Buffer
  - Band gap
  - Doping

- Numerical
  - Effective mass versus 6x6 k.p
  - Number of k.p points
  - k-vector range for k.p analysis
  - Method for separation between classical and quantum treatment
  - Integration method

Red indicates simulation parameters with high sensitivity.
Fitting Parameters, 40% SiGe Substrate

- **Dielectric (modeled as SiO$_2$)**
  - EOT, 38Å

- **Silicon**
  - Thickness, 47Å
  - Band splitting due to strain, 170 meV
  - Band gap, 920 meV
  - Band lineup compared to germanium, $\Delta E_v = 740$ meV

- **Germanium**
  - Thickness, 55Å
  - Band splitting due to strain, 105 meV
  - Band gap, not sensitive, 480 meV
  - Band lineup compared to relaxed SiGe buffer, 480 meV

- **Relaxed SiGe Buffer**
  - Band gap, not sensitive, 970 meV
  - Doping, $2 \times 10^{17}$ cm$^{-3}$

- **Numerical**
  - $6 \times 6$ k.p
  - Number of k.p points, 225 pts
  - k-vector range for k.p analysis, 0.30 (1/Å)
  - Method for separation between classical and quantum treatment, edge separation
  - Integration method, simple integration

**Red** indicates simulation parameters with high sensitivity.
Band Structure for 40% SiGe Substrate

At $V_G \sim 1.8$ V

38Å SiO$_2$  47Å s-Si  55Å s-Ge  500 nm 40% SiGe (p-type $2 \times 10^{16}$ cm$^{-3}$)

$E_G = 920$ meV  

$\Delta E_v = 740$ meV  

$E_{G,\text{eff}} = 180$ meV  

$480$ meV
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Sensitivity to $\Delta E_v$ between s-Si/s-Ge

- Simulation, $\Delta E_v = 740$ meV
- Experiment

$\Delta E_v - 25$ meV

$\Delta E_v + 25$ meV

Capacitance per Area (nF/cm$^2$)

Gate Voltage (V)
Sensitivity to effective band gap, $E_{G,\text{eff}}$

![Graph showing the relationship between gate voltage and capacitance per area. The graph indicates an inversion regime with a difficult experimental measurement. The effective band gap $E_{G,\text{eff}}$ is 180 meV.]
Sensitivity to effective band gap, $E_{G,\text{eff}}$
Sensitivity to effective band gap, $E_{G,\text{eff}}$

Many parameters affect this portion of the curve:
- Doping
- Ge thickness
- $E_{G,\text{eff}}$
- Ge valence band splitting
- SiGe band lineup to Ge
- DOS integration method

Difficult to decouple parameters for fitting.

Simulation, $E_{G,\text{eff}} = 180 \pm 60$ meV

Depletion Regime
Experimental and Simulated QSCV

Experimental Data for 60% SiGe MOS-Capacitors

Simulation, $\Delta E_v = 680$ meV, $E_{G,eff} = 190 \pm 60$ meV

Experiment

Capacitance per Area (nF/cm$^2$)

Gate Voltage (V)
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Summary of Extracted Values

- Extracted values given below

<table>
<thead>
<tr>
<th>Substrate</th>
<th>$\Delta E_v \pm 30$ (meV)</th>
<th>$E_G \pm 60$ (meV)</th>
<th>$E_{G, eff} \pm 60$ (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>40% SiGe</td>
<td>740</td>
<td>920</td>
<td>180</td>
</tr>
<tr>
<td>50% SiGe</td>
<td>760</td>
<td>950</td>
<td>185</td>
</tr>
<tr>
<td>60% SiGe</td>
<td>680</td>
<td>870</td>
<td>190</td>
</tr>
</tbody>
</table>

- The values for 50% SiGe are suspect
  - $E_G$ bigger than expected
  - Does not fall in line with trend
  - More materials analysis will be completed to verify strain, doping, and Ge fraction in substrate
Comparison to Theory

Suspect points for 50% SiGe, more materials analysis needed

Theory from Van de Walle and Martin using local density functional theory. Similar theoretical calculations by Van de Walle and Martin for the GaAs/AlAs band lineup have large discrepancies with experimental data.


Comparison to Theory and Past Work

Valence Band Offset of $s$-Si/$s$-Si$_{1-x}$Ge$_x$ on 40% Relaxed SiGe

- Chleirigh's Work
- This Experiment
- Theory, People and Bean

Line drawn only as guide
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Conclusions

- The valence band offset between s-Si/s-Ge is significantly larger (+100 meV) than theory by Van de Walle and Martin
  - $\Delta E_v = 740 \pm 30$ meV for 40% SiGe
  - Values are in good agreement with trend of Chleirigh’s work

- Determination of effective band gap less exact due to coupling of several different materials parameters
  - $E_{G,\text{eff}}$ found to be rather constant at $\sim 180-190$ meV for 40-60% SiGe substrates

- More materials analysis is needed to verify strain, doping, and Ge fraction in the samples
Increase in Band Gap Due to Quantum Confinement

- X-Valley CB in Silicon
  - 15 meV higher than band edge (effective mass approx.)
- Top VB in Germanium
  - 30 meV below band edge (6x6 k.p method)