Extraction of Energy Band Alignments in strained-Si/strained-Ge Type-II Heterostructures

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Different material systems can be used—(Mat. A/Mat. B) can be (InAs/GaSb) or (Si/Ge)—Si/Ge is investigated in current work.

Tunneling current is exponentially dependent on $E_{G,eff}$.

SS also depends on the electrostatics and $D_{it}$ at the oxide/semiconductor interface.

Both band alignment and $D_{it}$ can be explored with MOS-C structure.
MOS-Capacitor: Fabricated Structure

- Strained-Si/Strained-Ge pseudomorphic to relaxed SiGe layer
- varied Ge content to vary the strain
- MOS-C structure used to extract Valence band offset, $\Delta E_v$ and effective bandgap, $E_{G,\text{eff}}$
Valence Band Offset Extraction

Simulation for 35% SiGe MOS-C

Capacitance per Area (nF/cm²) vs. Gate Voltage (V)

I
II
III
IV

Simulation

Si   Ge   SiGe

I: high-k dielectric
II: high-k dielectric
III: high-k dielectric
IV: high-k dielectric
Extracting Key Parameters

Experimental Data (Quasistatic CV) for 35% SiGe MOS-C

Capacitance per Area (nF/cm²)

Gate Voltage (V)

EOT

Si thickness

$E_{G,\text{eff}}$ ($E_{G,s-Si}$)

$\Delta E_v$

I II III IV
Comparison of Best Fit Simulation and Measurement

Fitting Parameters:
\[ \Delta E_v = 770 \text{ meV} \]
\[ E_{(G, e f f)} = 190 \text{ meV} \]
\[ E_{(G, Si)} = 960 \text{ meV} \]
s-Si cap thickness = 49 Å
Al\(_2\)O\(_3\) thickness = 58 Å (38 Å EOT)
Sensitivity to $\Delta E_v$ between s-Si/s-Ge

- Simulation, $\Delta E_v = 770$ meV

CV technique is very sensitive to $\Delta E_v$!
Sensitivity to effective band gap, $E_{G,\text{eff}}$

- Simulation, $E_{G,\text{eff}} = 190$ meV
- Experiment

$E_{G,\text{eff}} - 25$ meV
$E_{G,\text{eff}} + 25$ meV

Capacitance per Area (nF/cm²)

Gate Voltage (V)
We find that $\Delta E_v$ is $\sim 100$ meV larger than theoretically predicted

$\therefore$ $E_{G,\text{eff}}$ between s-Si/s-Ge is 100 meV smaller than previously thought
Our extracted $\Delta E_v$ is inline with previous experimental work. Updated deformation potentials are required to correct theory.
Conclusions

• MOS-C structure emulates channel region of TFETs
• MOS-C analysis is a viable technique to extract band alignments in the Si-Ge system
  – Extracted $E_{G,\text{eff}}$ is $\sim 100$ meV smaller than predicted by theory
• Same band alignment information is required in III-V TFET heterostructures
• Technique still needs to be demonstrated in more difficult material systems
  – Currently pursuing MOS-C structures in the InAs/GaSb system
    • Important to extract $D_{it}$
Backup Slides
Motivation

• Tunneling current is exponentially dependent on effective band gap

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

- Simple MOS-C structure explores key components of the TFET
  - Dielectric/semiconductor interface
  - Tunneling junction, band alignment
  - Material quality

- Same extraction technique can be applied to III-V materials currently under investigation
Decoupling of Fitting Parameters

![Graph showing capacitance per area vs. gate voltage for different simulations and experiment.]

- High sensitivity to extraction of EOT and s-Si cap thickness.
Valence Band Extraction Method

Experimental Data for 35% SiGe MOS-C

- 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
As the Ge fraction of the relaxed SiGe substrate increases, strain in the s-Si layer increases and strain in the s-Ge layer decreases. The net result is that the Si CB and Ge VB (orange lines) end up moving in the same direction as strain is changed.
Summary of Extracted Values

Extracted values given below

<table>
<thead>
<tr>
<th>Substrate</th>
<th>$\Delta E_v$ (meV)</th>
<th>$E_{G,\text{eff}}$ (meV)</th>
<th>$E_G$ (meV)</th>
<th>S-Si cap thickness (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35% SiGe</td>
<td>770 ± 25</td>
<td>190 ± 50</td>
<td>960 ± 50</td>
<td>49 ± 2</td>
</tr>
<tr>
<td>42% SiGe</td>
<td>760 ± 25</td>
<td>185 ± 50</td>
<td>950 ± 50</td>
<td>45 ± 2</td>
</tr>
<tr>
<td>52% SiGe</td>
<td>670 ± 25</td>
<td>190 ± 50</td>
<td>870 ± 50</td>
<td>43 ± 2</td>
</tr>
</tbody>
</table>
Sensitivity to effective band gap, $E_{\text{G,eff}}$

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

Inversion Regime

Difficult experimental measurement
Sensitivity to effective band gap, $E_{G,\text{eff}}$

Depletion Regime

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

Experiment