Imaginary Band Structure and Its Role in Calculating Transmission Probability in Semiconductors

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Advisors: Judy Hoyt, Dimitri Antoniadis

Acknowledgements: Steve Laux (IBM)
Outline

• Introduction
  – Quantum mechanics refresher
  – Imaginary k-vector and WKB approximation
  – Imaginary band structure

• Applications of Imaginary Band Structure
  – Directional dependence of GIDL in MOSFETs
  – Strain dependence of tunneling current in Si tunnel diodes
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QM Transmission Through a Square Barrier

Classical Analogy

Potential Energy

Kinetic Energy

Trial Solution

\[
\psi(x) = \begin{cases} 
A_{x^+} \cdot e^{ik_1x} + A_{x^-} \cdot e^{-ik_1x}, & \text{for } x \leq 0 \\
B_{x^+} \cdot e^{ik_{II}x} + B_{x^-} \cdot e^{-ik_{II}x}, & \text{for } 0 \leq x \leq d \\
C_{x^+} \cdot e^{ik_{III}x}, & \text{for } x \geq d
\end{cases}
\]

Boundary Conditions

\[
\psi_I(0) = \psi_{II}(0) \\
\psi_{II}(d) = \psi_{III}(d) \\
\frac{d}{dx} \psi_I(0) = \frac{d}{dx} \psi_{II}(0) \\
\frac{d}{dx} \psi_{II}(d) = \frac{d}{dx} \psi_{III}(d)
\]

\[
V(x)
\]

\[
I \\
II \\
III
\]

incident wave, \( A_{x^+} \)

reflected wave, \( A_{x^-} \)

transmitted wave, \( C_{x^+} \)
Imaginary Momentum Vector

Plane Wave Solution
\[ \psi = C \cdot e^{ikx} \]

Momentum in the tunneling direction
\[ k = \sqrt{\frac{2m^*(E - V(x))}{\hbar^2}} \]

In the basic example of a plane wave tunneling through a square potential barrier, the momentum in the tunneling direction is imaginary inside the barrier which results in a decaying exponential.
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\[ \psi = C \cdot e^{ikx} \]

Momentum in the tunneling direction

\[ k = \sqrt{\frac{2m^*(E - V(x))}{\hbar^2}} \]

\[ \kappa \equiv \frac{k}{i} \]

\[ \psi = C \cdot e^{-\kappa x} \]
Tunnel Probability

- Start with the WKB approximation for tunneling probability

\[ T \sim \exp \left( -2 \int_a^b \kappa \, dx \right) \]
Start with the WKB approximation for transmission probability

\[ \kappa \equiv \frac{k}{i} \]

\[ T \sim \exp \left( -2 \int_{a}^{b} \kappa \, dx \right) \]

Action Integral
Constant Field Approximation

• For a constant field across the junction, action integral can be rewritten as

\[ \int_{a}^{b} \kappa \, dx = \int \kappa \frac{dE}{qF} \]

• Where \( F \) is the field, \( q \) is the charge of an electron, and \( E \) is energy. Since:

\[ qF \, dx = dE \]
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Assumes parabolic band

\[
\kappa = \sqrt{\frac{2m^*(E - V(x))}{-\hbar^2}}
\]
Constant Field Approximation

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\[ \kappa = \sqrt{\frac{2m^* (E - V(x))}{-\hbar^2}} \]

Can be calculated from imaginary band structure
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Full Band Structure of Silicon

Full Band Structure of Silicon

Full Band Structure of Silicon

The electric field provides energy for tunneling from valence band to conduction band.
Imaginary Band Structure
[100] Tunneling in Silicon

Imaginary Band Structure
[100] Tunneling in Silicon

Imaginary Band Structure

[100] Tunneling in Silicon

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GIDL in MOSFETs
(Gate Induced Drain Leakage)

**n-MOSFET**

1. **On State**
   - Thermionic emission of electrons
   - Energy band diagram

2. **Off State**
   - Tunneling of electrons
   - Energy band diagram

**n-TFET**

1. **On State**
   - Tunneling of electrons
   - Energy band diagram

2. **Energy Band Diagrams**
   - Conduction band
   - Valence band
Question:
What is the effect of channel orientation on GIDL?
GIDL Experiment

Simplified Tunneling Equation

General expression:

\[ T \approx \exp \left( -2 \int \kappa \frac{dE}{qF} \right) \]

For a triangular barrier:

\[ T \approx \exp \left( -\frac{4 (E_G)^{1.5}}{3 q |F| \hbar} \sqrt{2m_{\text{tunnel}}} \right) \]

<table>
<thead>
<tr>
<th>Tunneling Direction</th>
<th>Lobes with transverse electron mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>[100]</td>
<td>4</td>
</tr>
<tr>
<td>[110]</td>
<td>2</td>
</tr>
<tr>
<td>[111]</td>
<td>0</td>
</tr>
</tbody>
</table>

[100] Tunneling
4 lobes with transverse electron mass

[110] Tunneling
2 lobes with transverse electron mass

• <110> channel MOSFETs have about 10x GIDL current compared to <100> channel MOSFETs
GIDL Experiment Con’t

- <110> channel MOSFETs have about 10x GIDL current compared to <100> channel MOSFETs

Vertical tunnel diodes were fabricated on (100), (110), and (111) Si substrates to study tunneling along these directions.

Tunneling width determined by CV doping profile extraction and simulation.

GIDL Experiment Con’t

\[ T \approx \exp \left( -2 \int \frac{dE}{qF} \right) \]

- Dashed lines are curves calculated using a band edge effective mass
  - Band edge mass is insufficient in accurately calculating action integral
- Solid lines are calculated from the imaginary band structure
- Imaginary band structure is especially needed in analyzing tunneling in the [110] and [111] direction

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Strain Dependence of Tunneling in Vertical Silicon Tunnel Diodes

**Objective:** To determine the relative change in tunneling current due to applied uniaxial stress.

**Procedure:** Experimentally measure the uniaxially stressed vertical Si tunnel diodes and compare results to theoretical calculations.

Vertical tunnel diodes were fabricated on (100), (110), and (111) Si substrates to study tunneling along these directions.

The uniaxial bending apparatus was designed by the S. Thompson group at University of Florida.
IV Plot for (001) Wafer with [100] Stress

Thermal Regime (63mV/decade)

Tunneling Regime

Trap Limited Regime

Forward Bias

Voltage on N-Region (Volts)

Current (A)

Reverse Bias

Compressive Strain

Tensile Strain

Uniaxial Stress

[100] [110]

Tunneling Current
Relative Change in Current Compared to 0% Strain
(001) Wafer with [100] Stress

Increasing Compressive Strain

Increasing Tensile Strain
Imaginary Band Structure Calculation for Silicon (001) Wafer with [100] stress

- Analysis of the action integral calculated using imaginary band structure shows that the stress dependence is most sensitive to changes in band edge energies and occupancy of the bands.

\[ T \approx \exp \left( \int_{a}^{b} k_{x} \, dx \right) = \exp \left( \int_{a}^{b} \frac{dE}{qF} \right) \]
Theoretical Analysis

• Imaginary band structure calculations for (001) wafer with [100] stress showed a large sensitivity of the transmission probability to energy band edge movements with stress.
  – Little change in tunneling mass

• Strained imaginary band structure data was not available for all wafer/strain configurations

• Ultimately, the theoretical calculations were made without imaginary band structure calculations, taking into account the changes in band edge energy and occupation of the different lobes.
  – This produced a reasonable fit, since we compared changes in current with strain for a set tunneling direction.
  – Different tunneling directions were not compared to each other.
Relative Change in Current with Applied Strain

(a) (001) wafer, [100] strain
(b) (001) wafer, [110] strain
(c) (011) wafer, [100] strain
(d) (-110) wafer, [110] strain
Summary of the Tunneling Analysis

**[100] Stress**

- **E<sub>c</sub>**
- **x-lobe**
- **y-lobe**
- **z-lobe**

<table>
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<tr>
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<th>[011] tunneling</th>
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<td>x-lobe</td>
<td>m&lt;sub&gt;t&lt;/sub&gt;=0.19</td>
<td>m&lt;sub&gt;t&lt;/sub&gt;=0.19</td>
</tr>
<tr>
<td>y-lobe</td>
<td>m&lt;sub&gt;t&lt;/sub&gt;=0.19</td>
<td>m&lt;sub&gt;mixed&lt;/sub&gt;=0.32</td>
</tr>
<tr>
<td>z-lobe</td>
<td>m&lt;sub&gt;t&lt;/sub&gt;=0.98</td>
<td>m&lt;sub&gt;mixed&lt;/sub&gt;=0.32</td>
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\[
\frac{\Delta J}{J} \approx \frac{\Delta J_x}{J_{x0}} + \frac{\Delta J_y}{J_{y0}} > 0
\]

\[
J \approx J_x + J_y
\]

**[110] Stress**

- **E<sub>c</sub>**
- **x-lobe**
- **y-lobe**
- **z-lobe**

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\[
J \approx J_x + J_y
\]

**[100] Stress**

- **E<sub>c</sub>**
- **x-lobe**
- **y-lobe**
- **z-lobe**

**[001] wafer, [100] strain**

- Theoretical
- Experimental

**[110] wafer, [100] strain**

- Theoretical
- Experimental
Summary

• Imaginary k-vector, $\kappa$, represents a decaying exponential wavefunction

• Imaginary band structure calculations allow for accurate calculation of the action integral
  – Band edge effective mass is insufficient to capture tunneling in different directions

• Band structure calculations that incorporated strain matched the trending behavior of relative change in tunneling current vs strain
Acknowledgements

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