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Theory and design of (111) oriented Si/SiGe quantum cascade lasers

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Overview



- Conduction band structure
- QCL design
- Transport calculations
- Waveguide modelling and gain

(001) conduction band



Bulk Si/SiGe band edge in 6 valleys (for Ge < 85%)

QCL design complicated due to:

- Strain → different energies for valley sets (perpendicular & in-plane)
- Anisotropy → different effective masses for valley sets
- Perp. effective mass ≈
 0.92 m_e → small oscillator
 strength





Conduction band offsets

Usable (001) band offset limited [2]:

 Deep quantum wells for perp. valleys. (ΔV ≈ 400 meV)

 \rightarrow Strongly bound states

- But, shallow wells for inplane valleys overlap
 - → Strong optical absorption
 - → Leakage currents
- QCL design limited to energies below in-plane valleys



[2] A. Valavanis *et. al.*, Phys. Rev. B **78**, 035420 (2008)

(111) conduction band





[1] S. Smirnov & H. Kosina, Solid-State Electron. **48**, 1325 (2004)

Many problems solved by moving to (111) orientation:

- Identical valley crosssections
 - → All valleys at same energy
 - → All effective masses identical
- Smaller quantisation effective mass ≈ 0.26 m_e [1]
 - → larger oscillator strength







- (001) energy range limited by strain splitting between valley sets
 - → Large substrate Ge content desirable
- But ~10% Ge needed for mechanical stability
 - → Usable energy range ~ 50 meV
- No strain splitting between valleys in (111) orientation
 - → Band offset increases with barrier Ge fraction
 - \rightarrow 50% Ge barriers give 150 meV band offset

Bound to continuum QCL design



5.2 THz, seven well design

- Optical transition between bound state and continuum states
- Si wells/Si_{0.6}Ge_{0.4} barriers
- n-type doping of 5×10¹⁶ cm⁻³ throughout (modulation doping may be poor)
- Designed for 7.4 kV/cm applied electric field
- 10% Ge virtual substrate for strain balance





Scattering rates used to determine populations:

- Time independent perturbation model of scattering
- Self-consistent solution of rate equations gives populations

Population inversion achieved:

- Fast Coulombic scattering depopulates miniband
- Long upper laser level lifetime:
 - Si wells minimise alloy disorder scattering
 - Low Ge barriers reduce interface roughness
 - Optical transition (20 meV) below phonon energy (43 meV)

Current density





- Current density peaks at design field due to band alignment
- Low temperature peak of 2 kA/cm²
- Current increases with temperature due to faster scattering

Waveguide modelling



2D finite element modelling of modal overlap:

Surface plasmon waveguide:

- Poor confinement, Γ =17%
- Low waveguide losses a_w=10 cm⁻¹
- High threshold gain:

$$g_{\mathrm{TH}} = rac{a_{\mathrm{w}} + a_{\mathrm{m}}}{\Gamma} = 68 \ \mathrm{cm}^{-1}$$



Double-metal waveguide:

- *Γ*=100%
- Threshold gain of 31 cm⁻¹



Gain spectrum

- Calculated at 7.4 kV/cm applied electric field
- Peak at 5.2 THz
- Other peaks due to transitions to lower energy subbands
- •Gain decreases with temperature due to
 - Linewidth broadening
 - Reduced population inversion
- Gain exceeds losses up to 105 K



Conclusions



(111) oriented Si/SiGe is a good candidate for THz QCLs

- Low effective mass: $m_q = 0.26 m_e$
- Large usable band offset: $\Delta V \sim 150 \text{ meV}$
- Net gain predicted for bound-to-continuum laser
- 5.2 THz emission
- Double metal waveguide has gain threshold of 31 cm⁻¹
- Gain predicted up to 105 K

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