Conference or Workshop Item:

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

A. Valavanis*, L. Lever, C. A. Evans, Z. Ikonić and R. W. Kelsall

* a.valavanis05@leeds.ac.uk

Overview

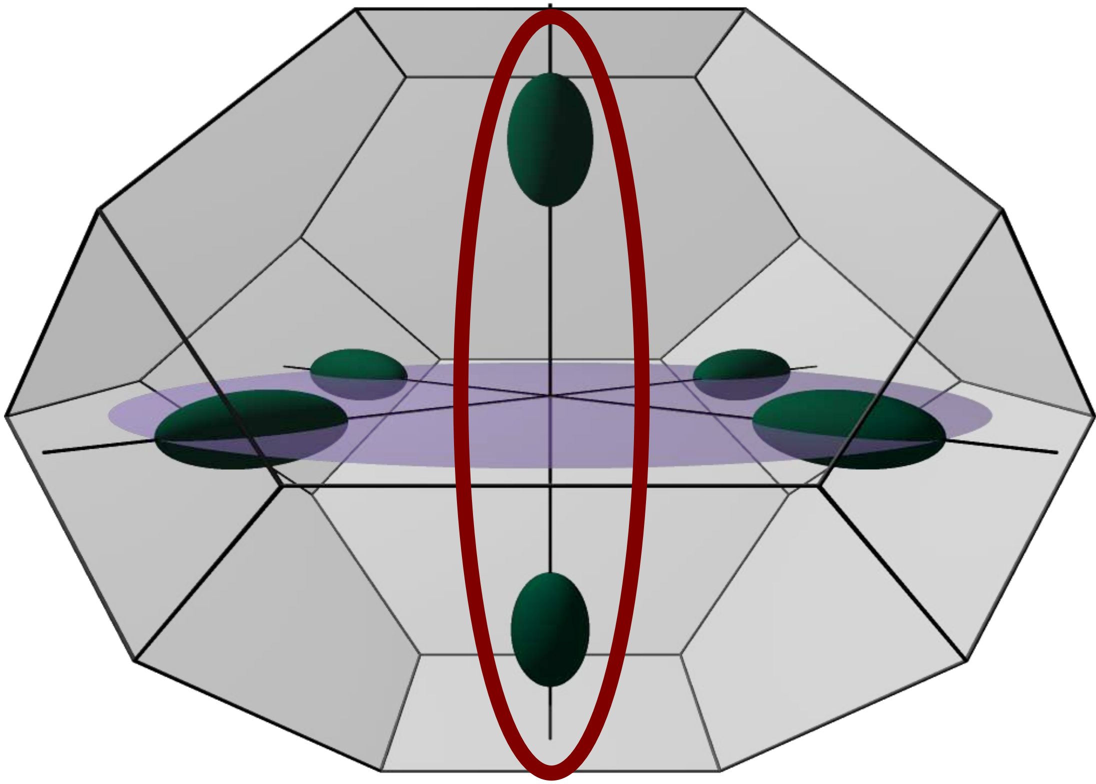
- Conduction band structure
- QCL design
- Transport calculations
- Waveguide modelling and gain

(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)

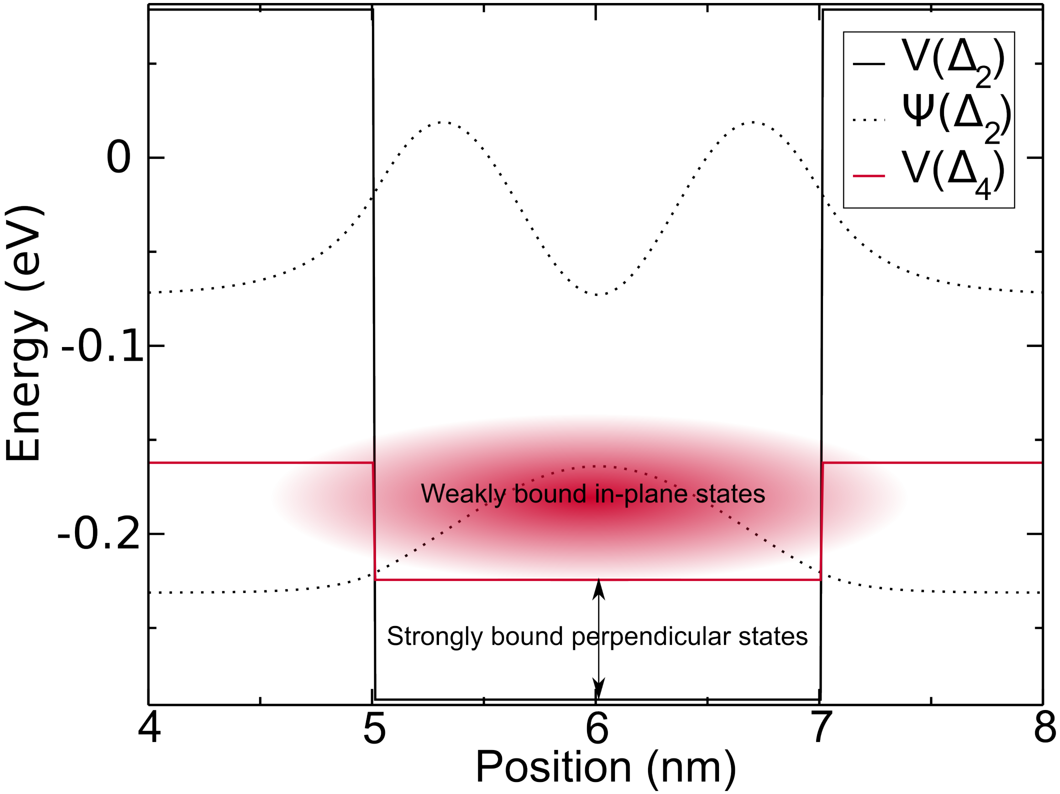
  → **Strongly bound states**

- **But**, shallow wells for in-plane valleys overlap

  → **Strong optical absorption**

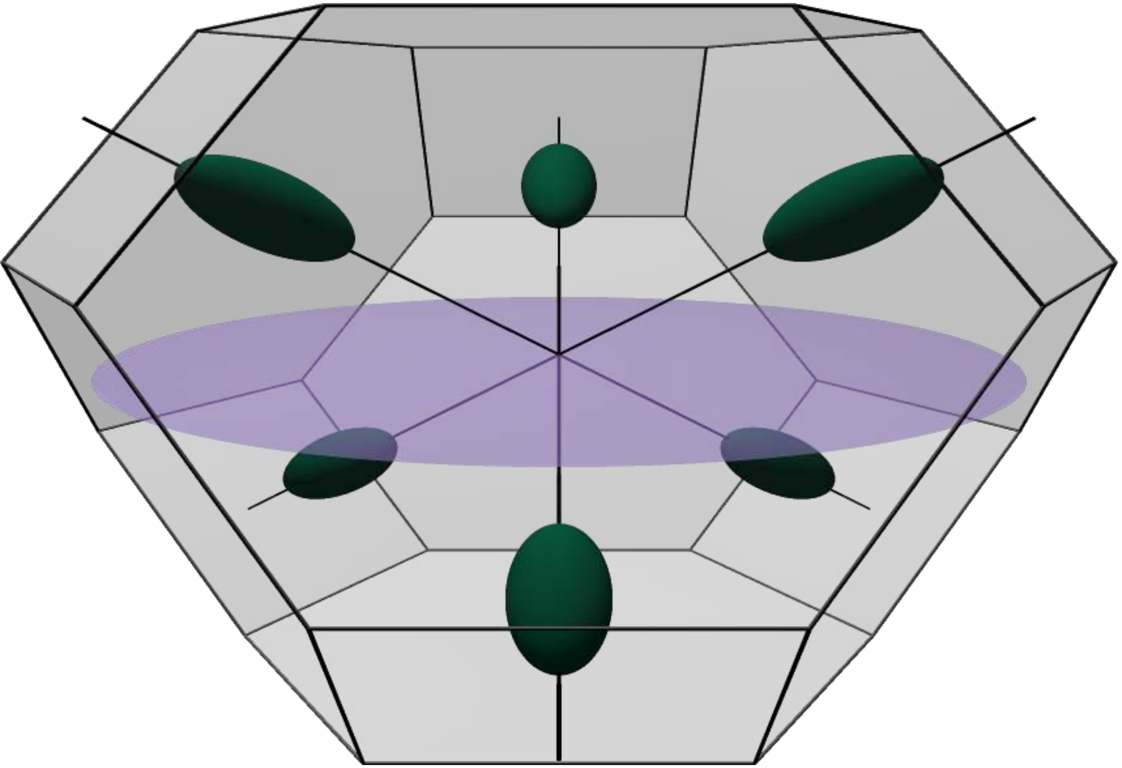
  → **Leakage currents**

- QCL design limited to energies below in-plane valleys



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

(111) conduction band



Many problems solved by moving to (111) orientation:

- Identical valley cross-sections

  → **All valleys at same energy**

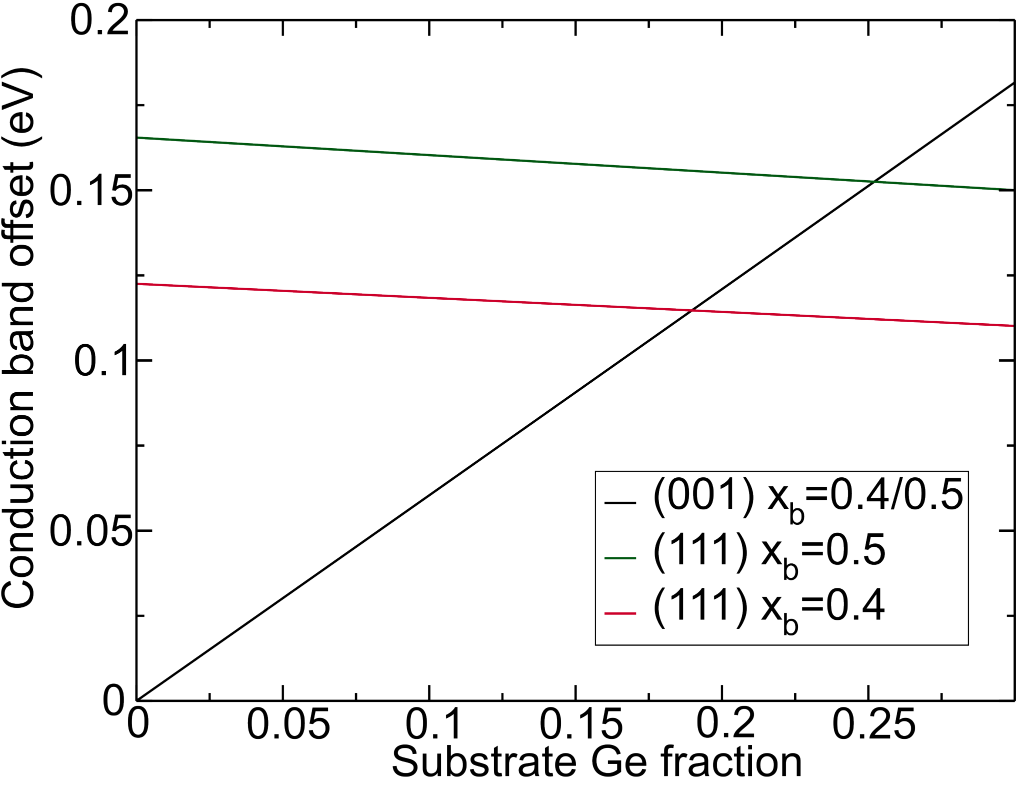
  → **All effective masses identical**

- Smaller quantisation effective mass ≈ 0.26 m_e [1]

  → **larger oscillator strength**

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

Conduction band offsets



- (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

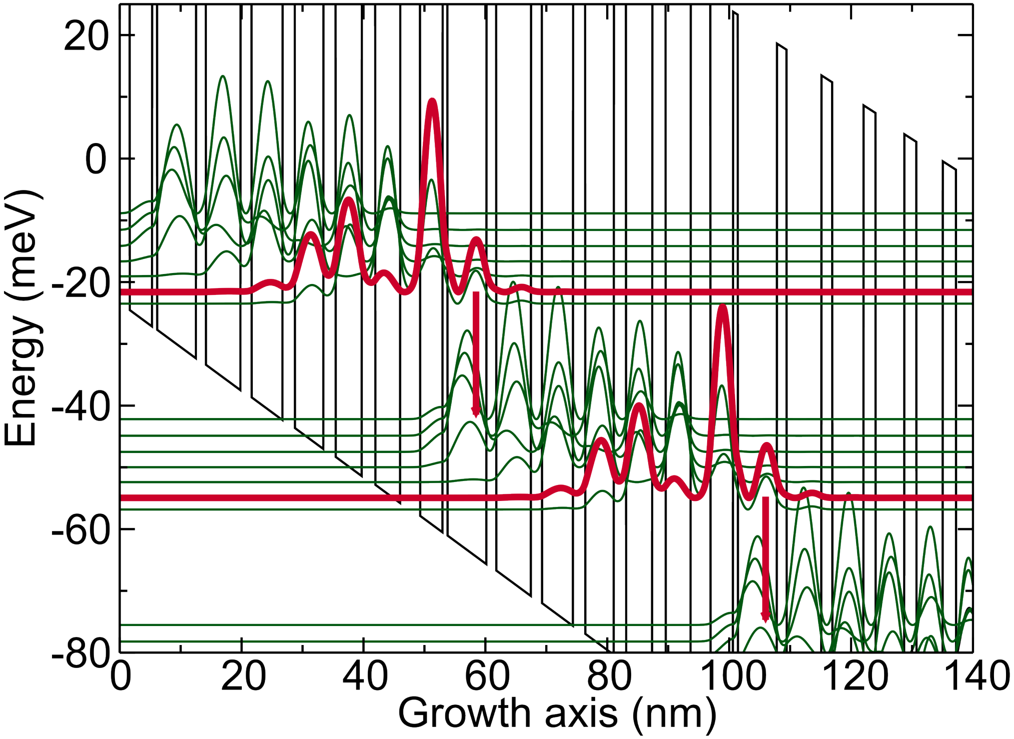
  → **Band offset increases with barrier Ge fraction**

  → **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 5×10^{16} cm^{-3} throughout (modulation doping may be poor)
- Designed for 7.4 kV/cm applied electric field
- 10% Ge virtual substrate for strain balance



Transport modelling

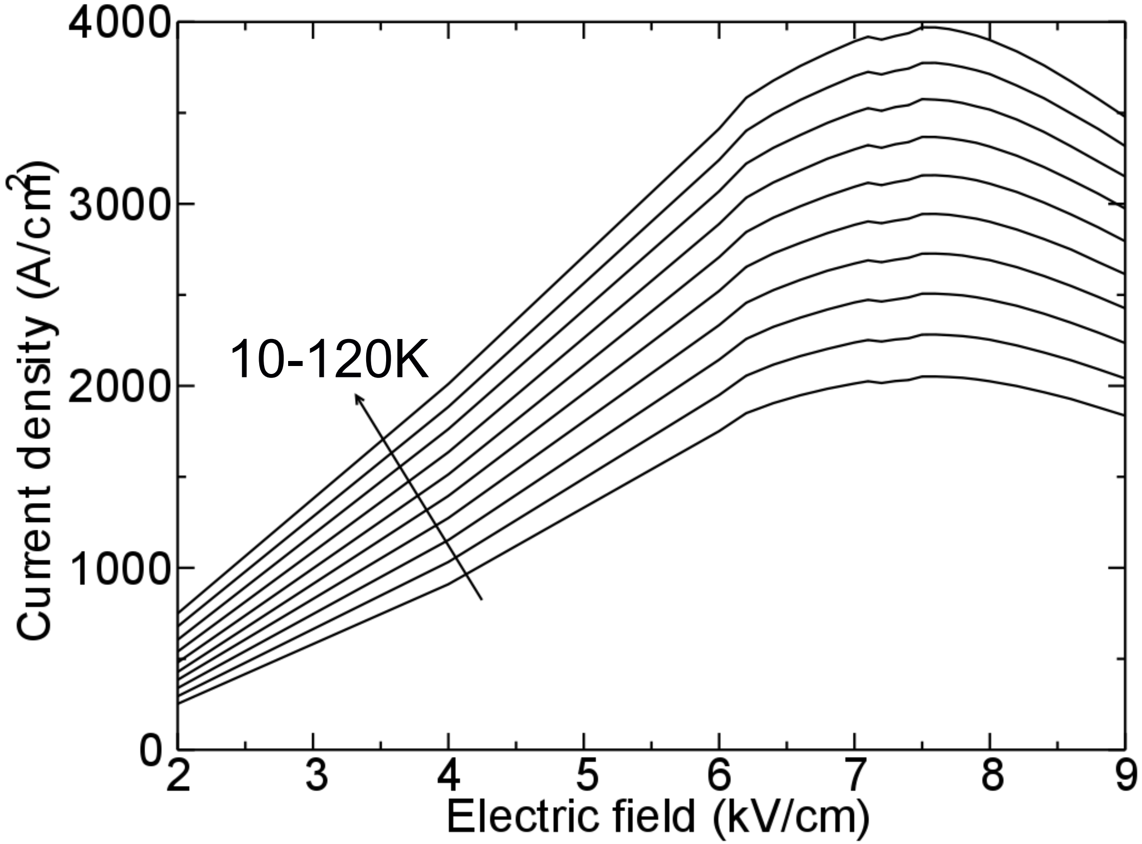
Scattering rates used to determine populations:

- 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

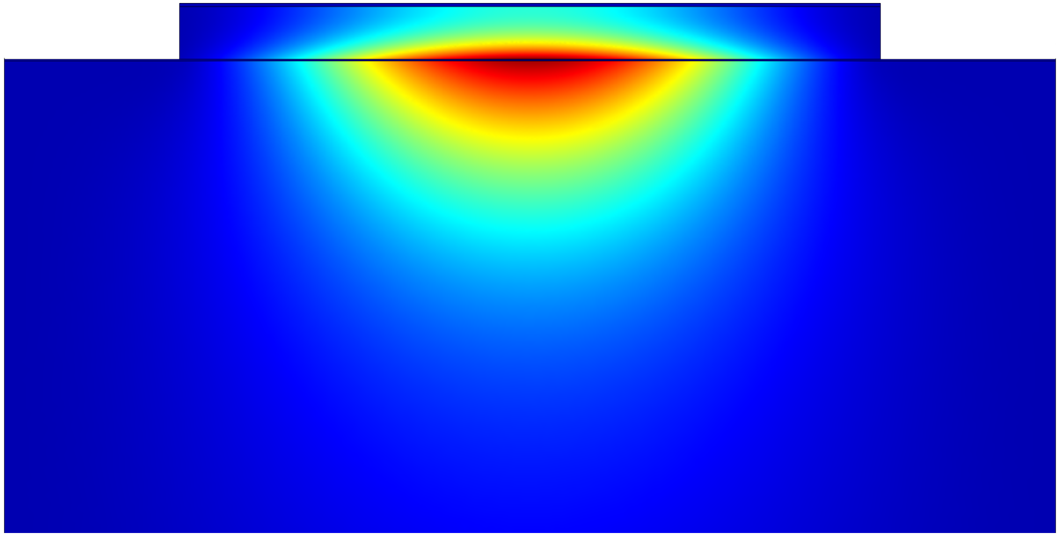


- Current density peaks at design field due to band alignment
- Low temperature peak of 2 kA/cm^2
- Current increases with temperature due to faster scattering

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:

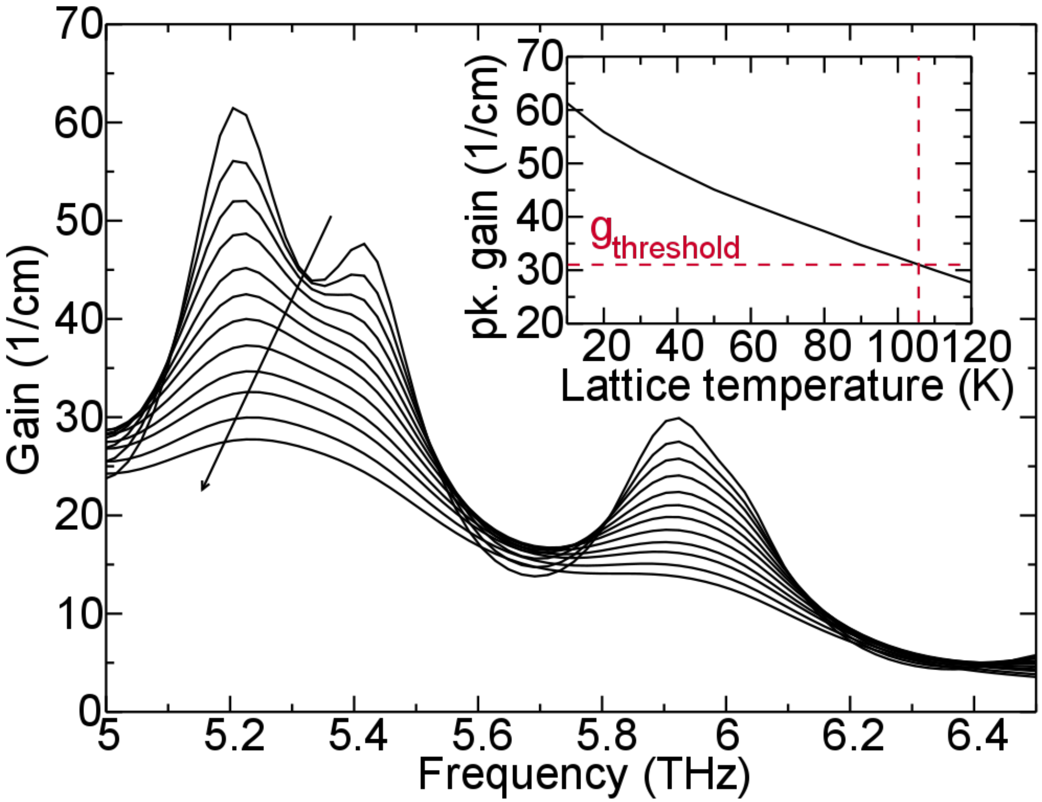
$$g_{TH} = \frac{a_w + a_m}{\Gamma} = 68\ \text{cm}^{-1}$$

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: $\Delta V \sim 150$ 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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