n-type Si/SiGe quantum cascade structures

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Advantages of n-type Si/SiGe

QCLs typically use III-V materials. Si/SiGe could offer:

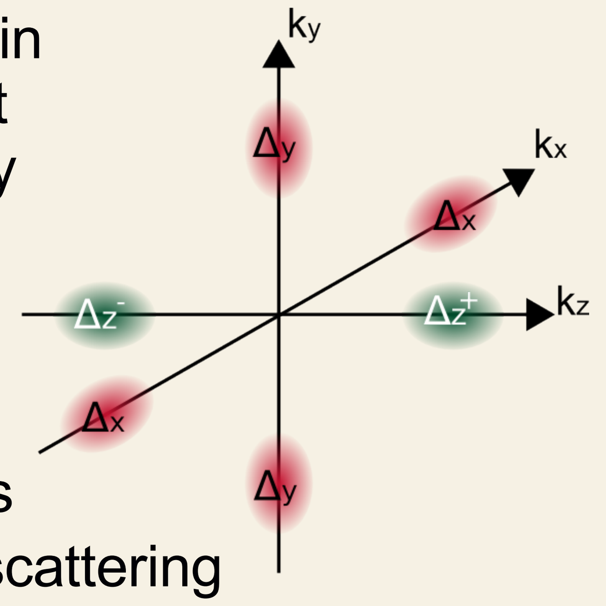
- Integration with CMOS for system-on-a-chip applications
- Cheaper processing

Si/SiGe QCL research so far has used p-type materials. n-type could solve several problems:

- Simpler band structure: almost parabolic band edge gives smaller transition linewidths than p-type systems
- No light-hole to heavy-hole optical transitions
- Negligible interband mixing (1-band effective mass approximation (EMA) acceptable)

Design challenges

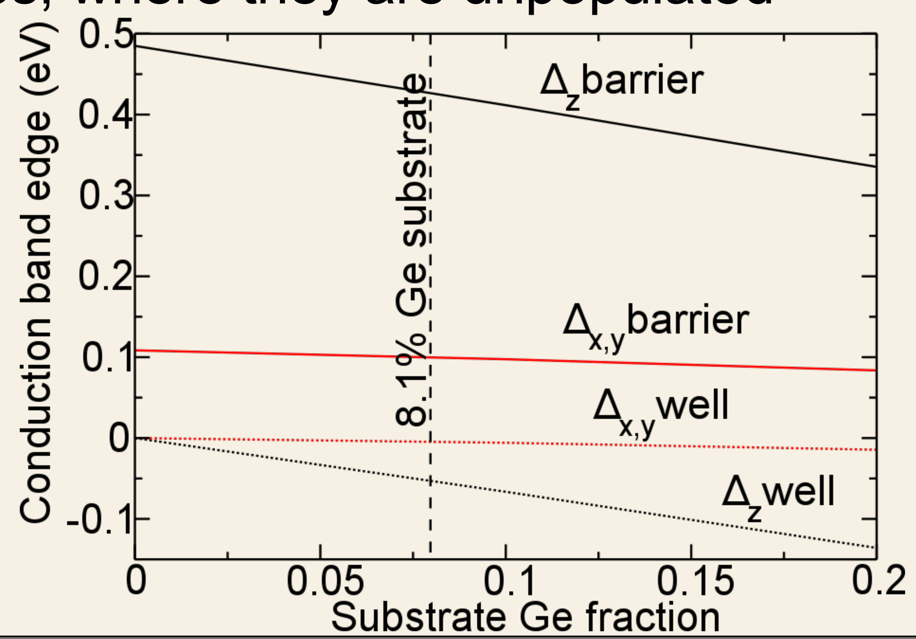
- Conduction band minima in Δ valleys (although indirect band gap is not necessarily a problem)
- For growth in z direction, strain and effective mass anisotropy split these into two Δ_z and four $\Delta_{x,y}$ valleys



- No resonant LO phonon scattering
- Poor modulation doping control
- Diffuse interfaces
- Large Δ_z effective mass and strong confinement give low wavefunction overlap

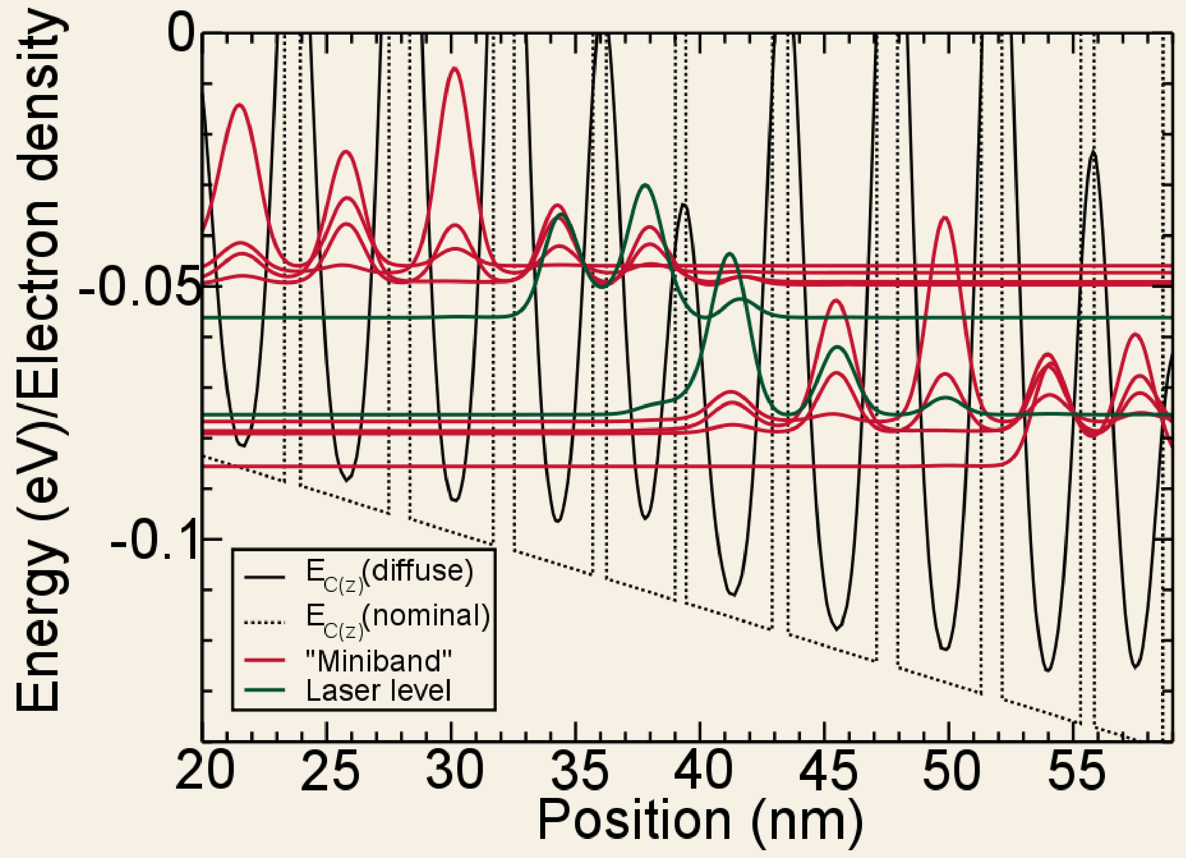
Si/SiGe band offsets

- Plot shows conduction band potential for the Si wells and $Si_{0.4}Ge_{0.6}$ barriers in proposed structure
- 8.1% Ge substrate required for strain balance
- Increased strain shifts $\Delta_{x,y}$ states to high energies, where they are unpopulated



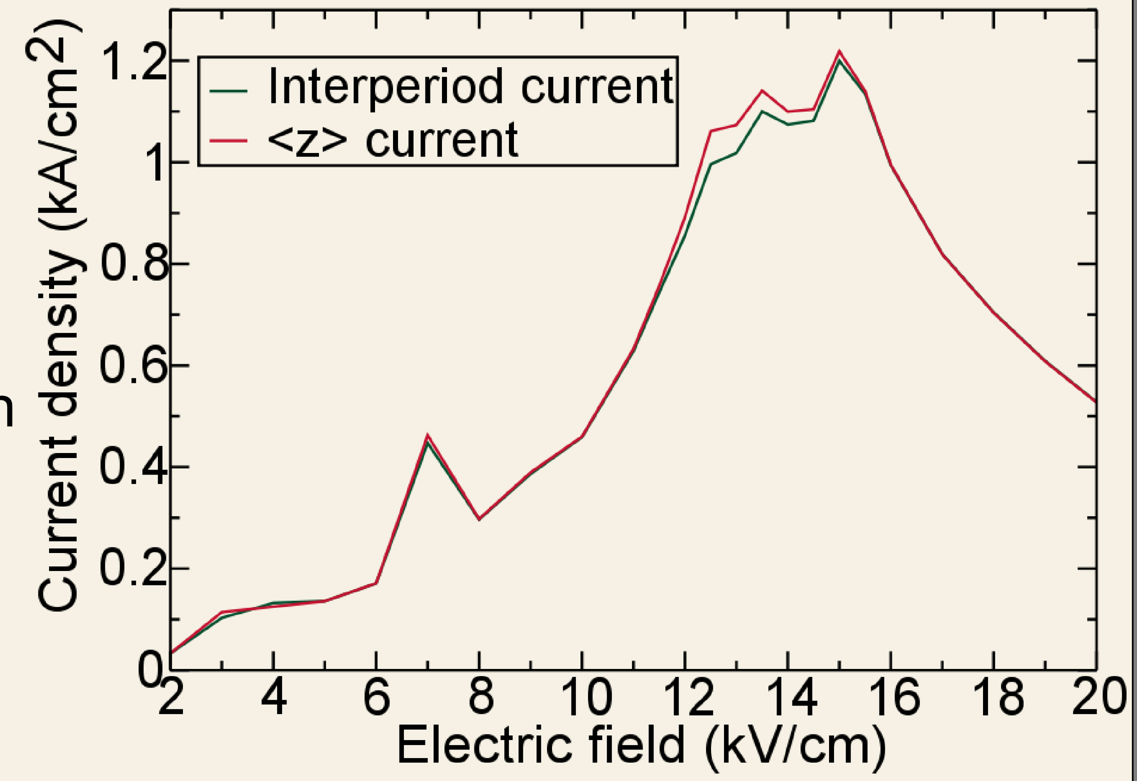
Quantum Cascade (QC) device design

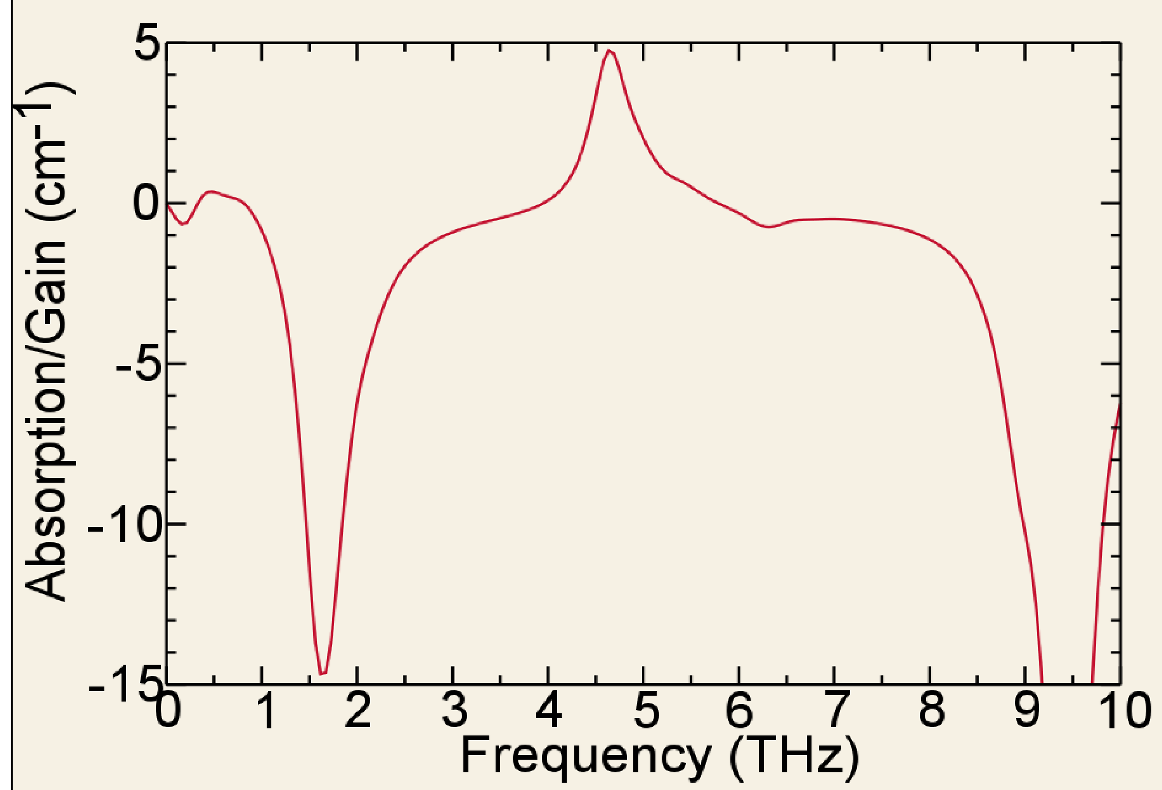
- 5 wells per period: $Si_{0.4}Ge_{0.6}$ barriers (underlined) and Si wells with thickness of 0.35, 3.5, 0.6, 3.6, 0.8, 3.4, 0.8, 3.2, 0.5, 2.8 nm
- 1nm Ge interdiffusion length assumed
- Designed for 15 kV/cm electric field
- Lower laser level is at top of "miniband": Rapid depopulation into upper laser level of next period
- n-type doping of 2×10^{16} cm^{-3} throughout, as modulation doping control is poor
- Simulated under envelope function/EMA at lattice temperature of 4K



Simulated performance

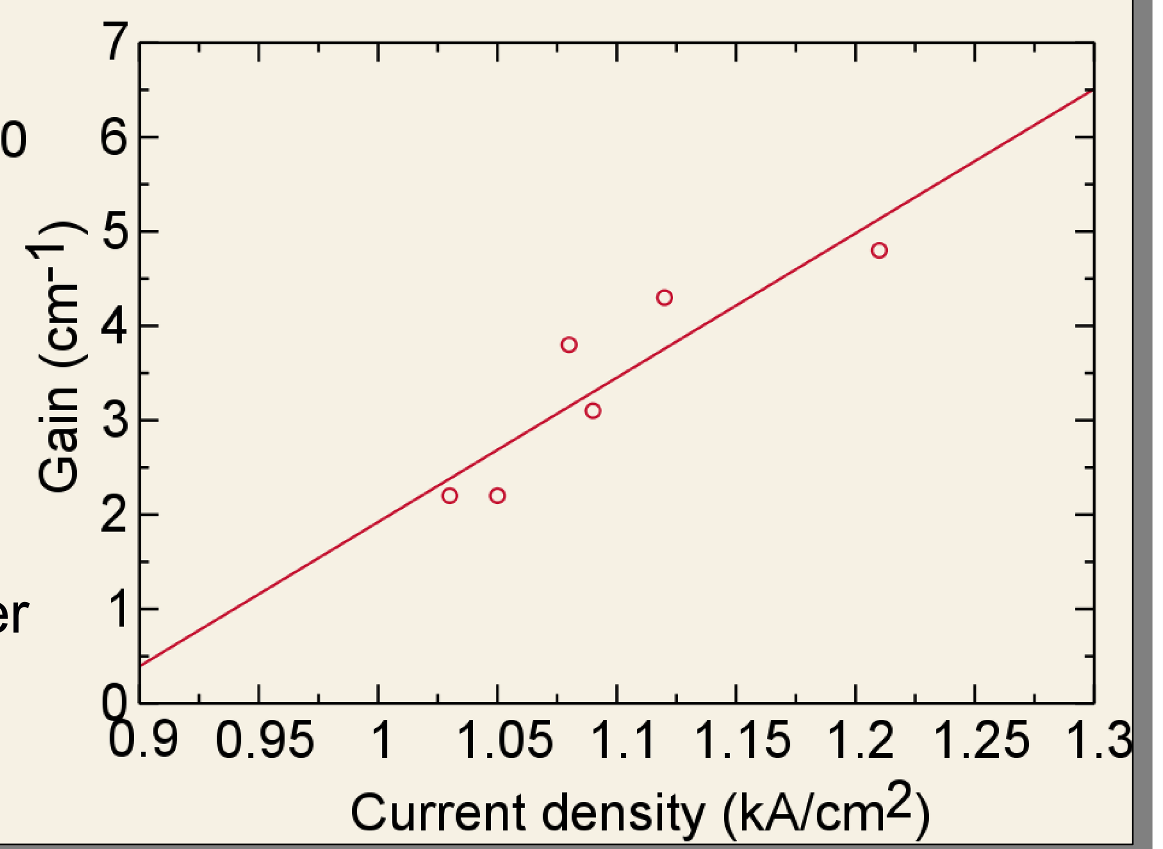
- Assumptions of initial and final electron positions needed for current. Either:
  - Centre of period or
  - Expectation position for state
- Maximum current density ~1.2 kA/cm^2 corresponds to optimal "miniband" formation at 15 kV/cm





- Maximum gain of 4.7 cm^{-1} at 4.6 THz,
- Absorption peaks due to optical transitions within "miniband" and to higher energy states

- Electron mobility of 25 cm^2/Vs at 15 kV/cm due to incoherent transport
- Sheet doping of 3.9×10^{10} cm^{-2} yields low Poisson shift in conduction band potential
- Electron temperature of 150 K assumed
- Drude model for bulk Si predicts free carrier losses of 15 cm^{-1}. However, this is a poor approximation to heterostructure carrier dynamics



Scattering mechanisms

Populations are calculated from self-consistent rate equations including alloy disorder (AD), interface roughness (IR), electron-phonon (EP), electron-electron (EE) and ionized impurity (II) scattering mechanisms.

II and EE scattering dominate between subbands which are close in energy. This rapidly depopulates the lower laser level and provides population inversion. Conversely, AD and EP scattering increase with energy separation, limiting population inversion between widely separated states.

$\Delta_z \rightarrow \Delta_{x,y}$ EP scattering is slow when $\Delta_{x,y}$ states are at high energies. Hence population of $\Delta_{x,y}$ subbands is negligible.

Conclusions

- n-type Si/SiGe QCLs offer several possible advantages over both III-V materials and over p-type Si/SiGe designs
- May be realisable, although challenges remain
- Large Δ_z conduction band offsets are achievable
- $\Delta_{x,y}$ states can be strain shifted to high energies, and hence their populations are reduced
- Ge interdiffusion causes significant changes to the system
  - Barrier heights reduced
  - AD scattering increased
  - IR scattering reduced
- Population inversion achieved by intra-"miniband" scattering
- Net active region gain predicted, although possibly not enough to overcome free carrier losses
  - Large longitudinal effective mass limits wave function overlap and hence gain
  - Thin barriers required
- Alternative approaches may resolve some issues associated with high longitudinal effective mass or strain splitting. Candidates include:
  - [111] orientated Si-rich systems
  - L-valley transitions in Ge-rich systems

Related publications

[1] I. Lazic *et. al.*, J. Appl. Phys. **101**, 093793 (2007).
[2] S. A. Lynch *et. al.*, IEEE J. Sel. Top. Quant. **12(6)**, 1570 (2006)
[3] Z. Ikonic *et. al.*, J. Luminescence **121**, 311 (2006)
[4] G. Dehlinger *et. al.*, Science **290(5500)**, 2277 (2000)
[5] J. Zhang *et. al.*, J. Crystal Growth **278**, 488 (2005)