The effects of interdiffusion in Si/SiGe THz quantum cascade devices

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Overview

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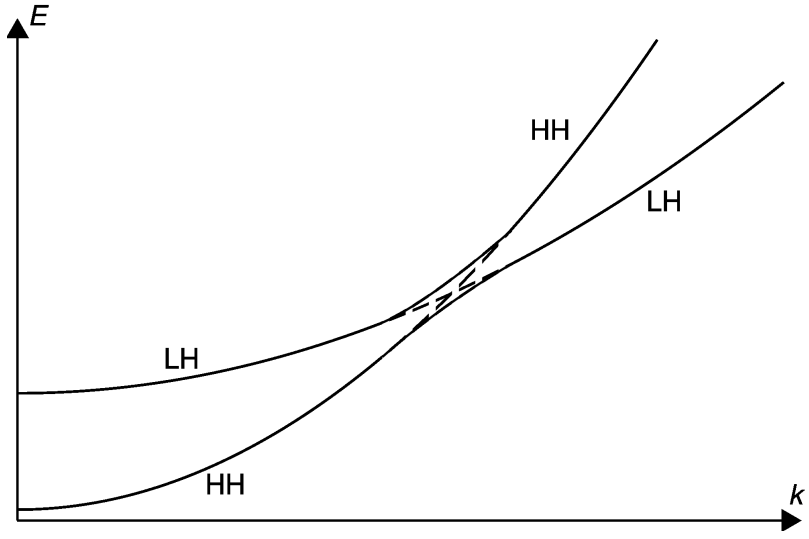
- In the modelling of heterostructures for intersubband lasers we generally assume abrupt interfaces
- Usually consider GaAs/AlGaAs
- Si/SiGe structures have much higher effective masses
- (So spatial extent of wavefunctions will be reduced)
- Dimensions of structures will therefore be smaller
- Ge more mobile than Al in GaAs/AlGaAs
- Effects of interdiffusion expected to be more significant

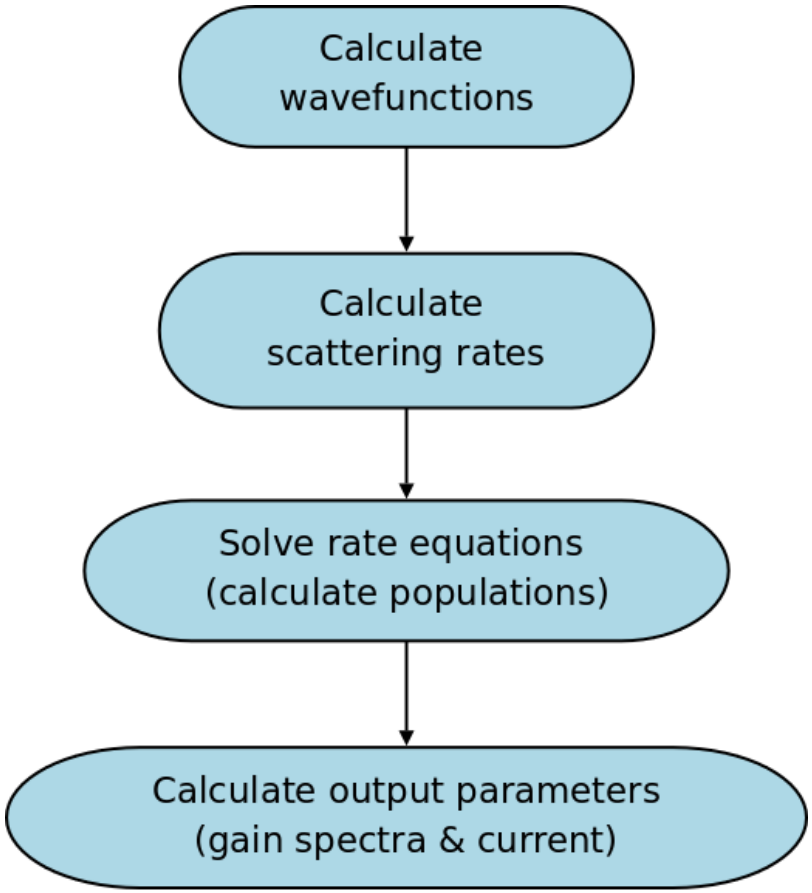
p-type Si/SiGe QCLs

- $m^* = 0.49\, m_0$ (HH)
- $m^* = 0.16\, m_0$ (LH)
- Strain splits light- and heavy-hole states
- LH higher in energy (upside-down energy picture)
- Non-zero k-vectors, LH and HH mix
- QCL design philosophy: push light-hole states to higher energies



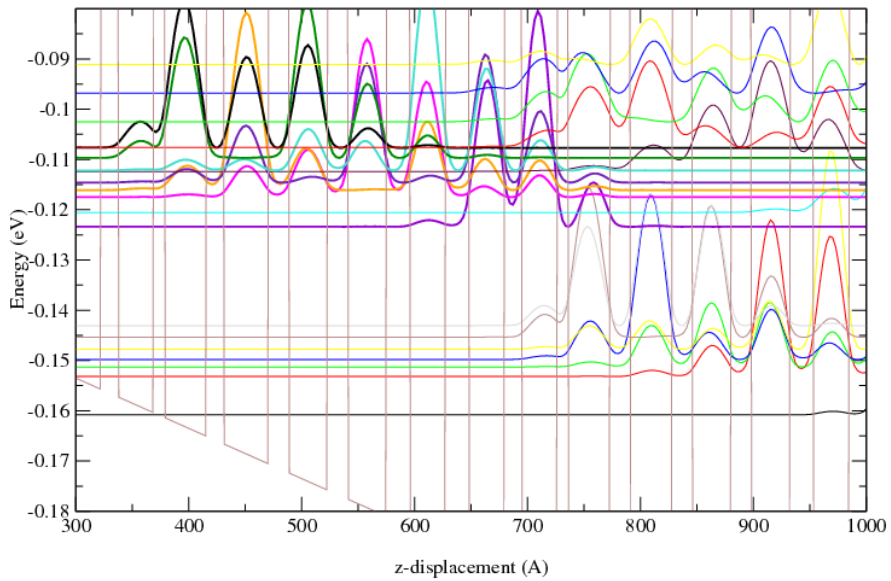
Simulation model

- 6x6 k.p bandstructure calculation
- Numerical solution of Schrödinger equation
- Scattering rates for: alloy disorder, interface roughness, carrier–carrier, ionised impurity, acoustic & optical phonons
- Assume Fermi distribution of carriers within subbands
- Solve rate equations self-consistently to calculate subband populations



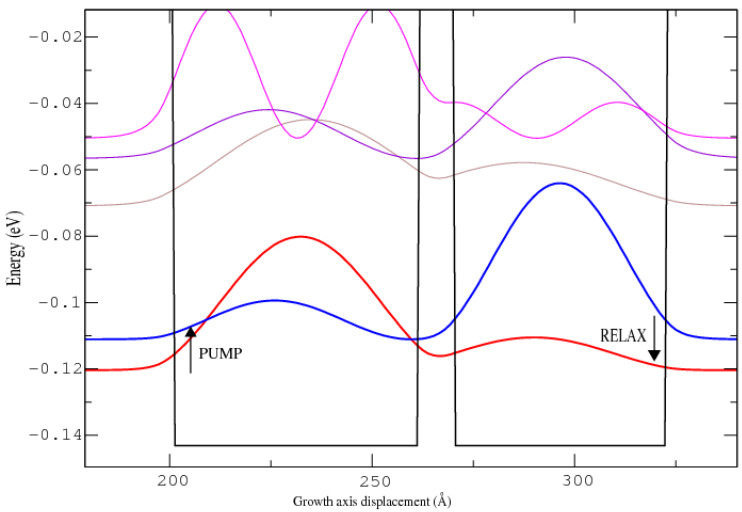
p-type Si/SiGe QCLs

- THz (15 meV) transition, so can push LH states to energies above the upper laser level (unlike MIR)
- For a strain symmetrised system with Si barriers, need 50% Ge fraction wells (available with gas source MBE)
- Higher energy barriers therefore must be thin
- Ge diffuses into Si layers
- Are abrupt interfaces a good approximation?



Pump–Probe Data

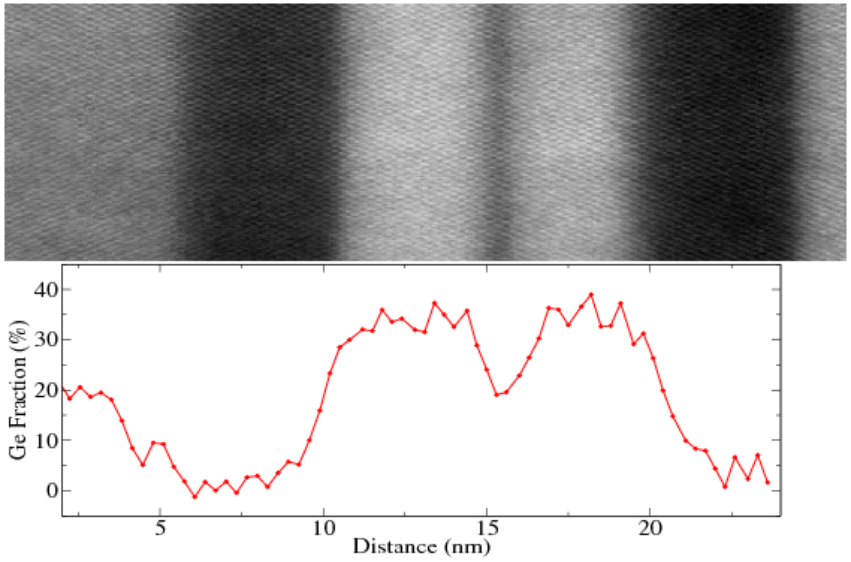
- 2 well structure grown for pump-probe measurements using the FELIX free electron laser facility at Utrecht
- $Si_{0.6}Ge_{0.4}$ wells, Si barriers.
- Measured dimensions for wells: 61 ± 0.6 Å and 52 ± 0.6 Å, with the barrier thickness 8 ± 0.6 Å
- Calculated separation of states $= 9.5$ meV
- Measured $= 15 \pm 1$ meV
- Why this discrepency?



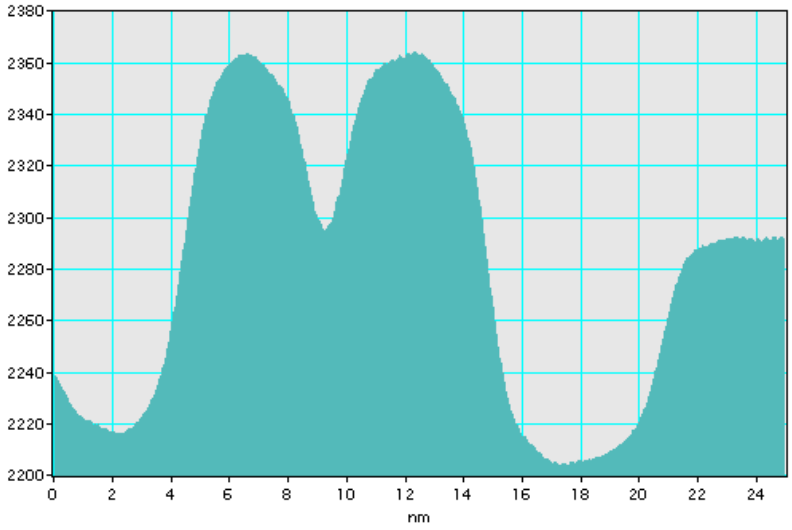
SuperSTEM data

- aberation corrected superSTEM facility at Daresbury, UK. Data indicates interfaces may be diffuse
- EELS gives an intensity proportional to the atomic number
- Nominally pure Si barriers may actually contain significant Ge fraction
- Suggests interdiffusion of Si/SiGe may have significant effect on bandstructure

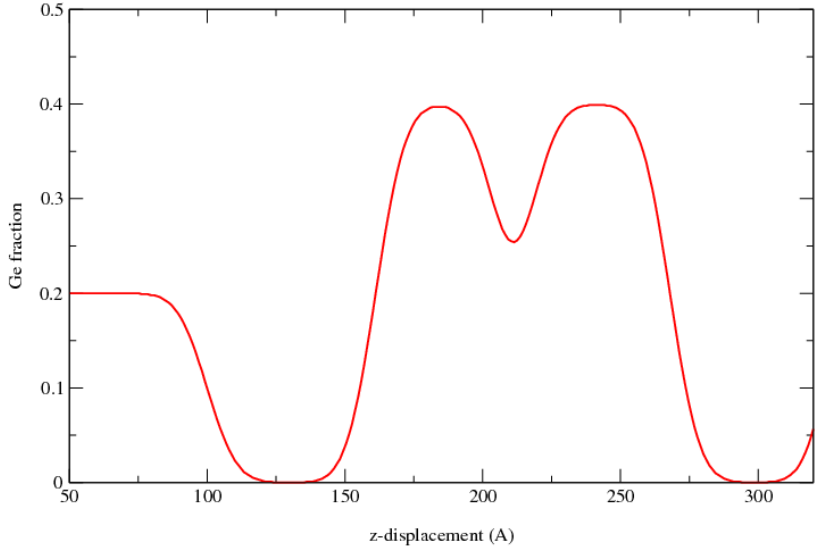
Electron energy loss spectra (EELS)



SuperSTEM data



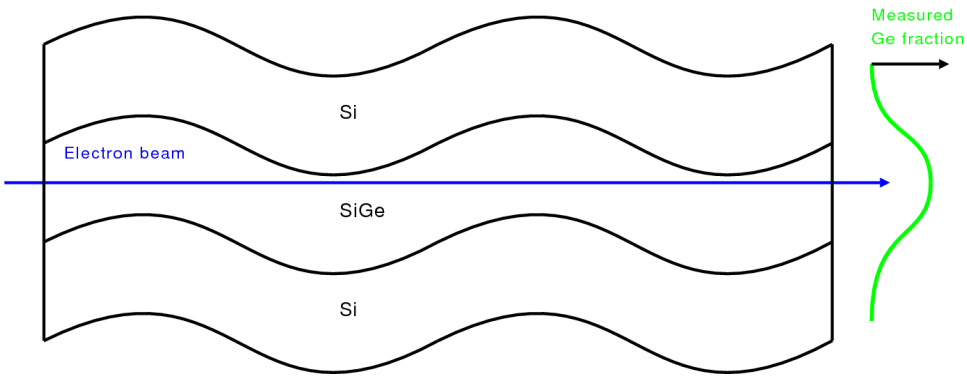
ADF profile



1.2 nm diffusion length,
error-function interdiffusion

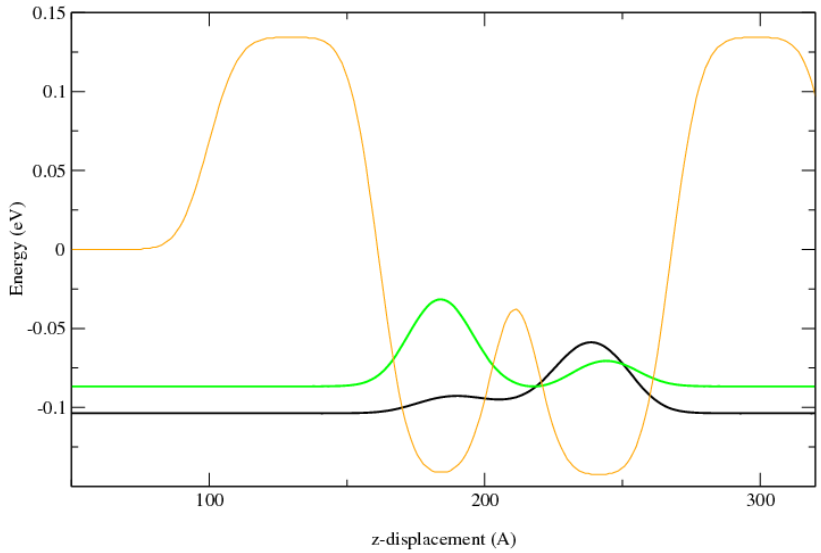
A word of caution...

- TEM data likely to overestimate interdiffusion
- Interface roughness can produce the same artefacts
- Thankfully we have more to go on...



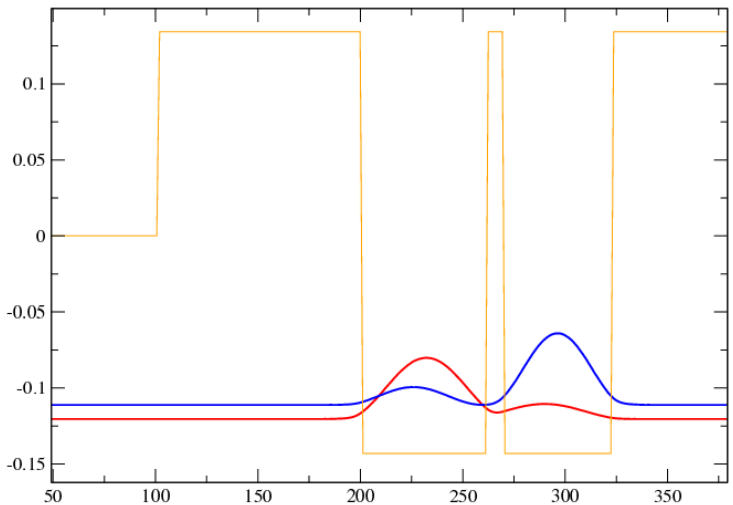
Effect of interdiffusion

- 1 nm diffusion length
- Error function diffusion
- State separation = 15.4 meV (in agreement with pump-probe data)
- (Nominally pure) Si barrier now greatly reduced in energy



Effect of interdiffusion

- Inclusion of the interdiffusion significantly alters band edge profile
- Wavefunctions change too
- Thin barriers become lower in energy
- In (low μ) SiGe systems, thin barriers are desired.



QCL wavefunctions

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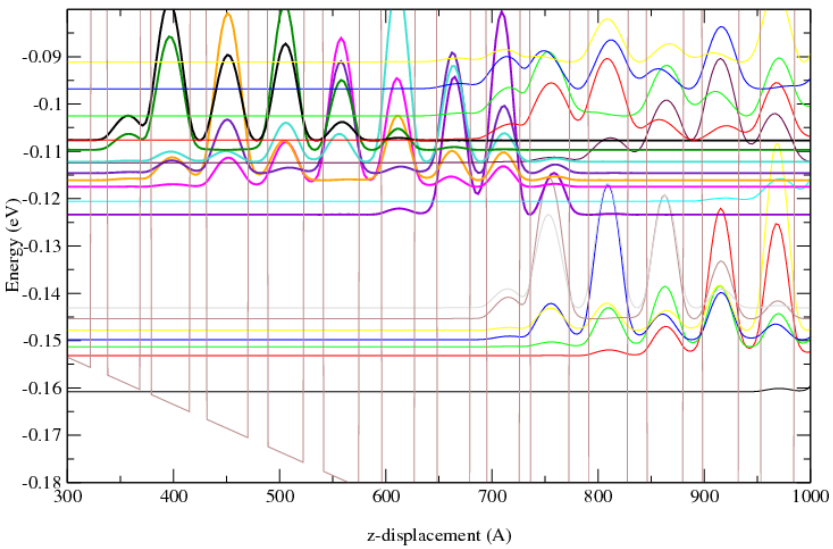
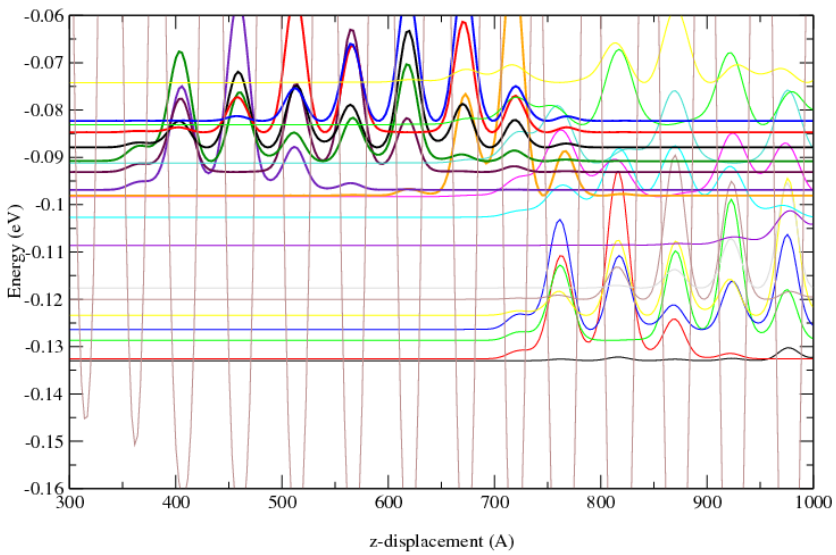


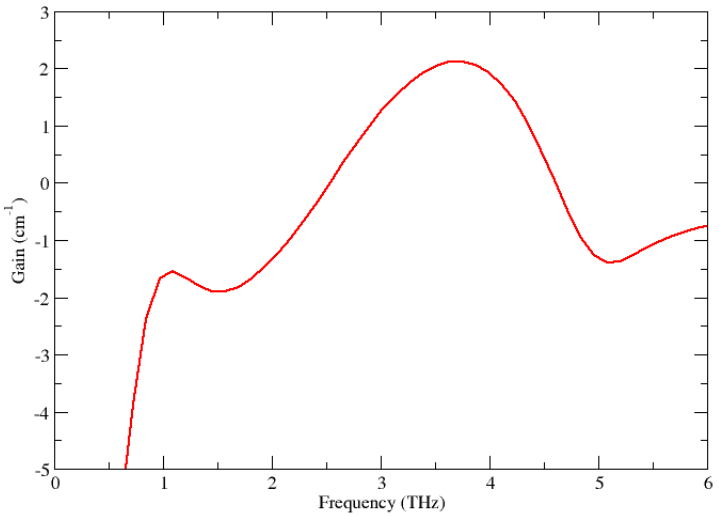
Existing *p*-type design



With interdiffusion

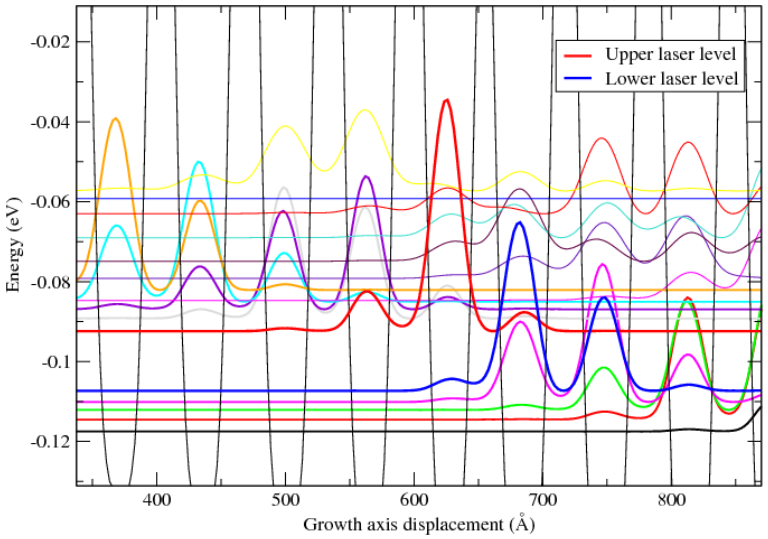
Gain spectra

- Gain is lost for simluation with interdiffusion
- We just see a large broadband absorption
- Interdiffusion is clearly a significant design issue
- However, we can incorporate this into the design...

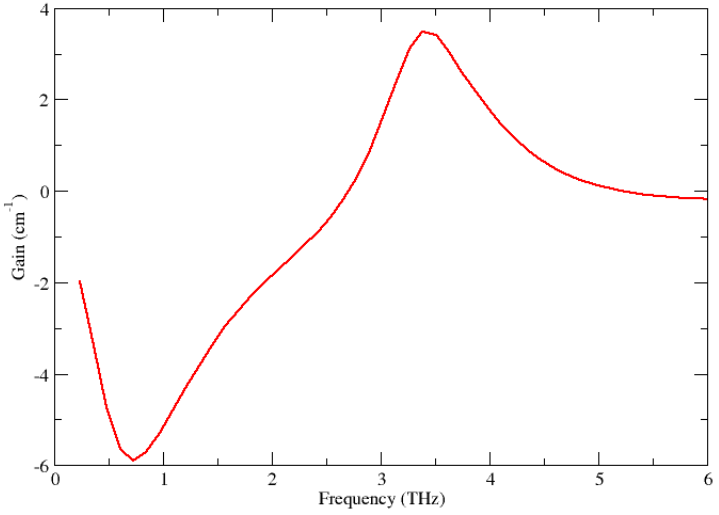


Gain spectra for original design

Effect of interdiffusion



New design including interdiffusion



Simulated performance is similar to previous design

Conclusions & future work

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- TEM data indicates Si/SiGe interdiffusion over approx. 1 nm
- Energy eigenstates with 1 nm diffusion length match pump–probe measurements
- Existing designs are sensitive to this interdiffusion
- Designs can be modified to account for the interdiffusion, with similar simulated performance
- The *p*-type QCL structures discussed here have all been grown at Imperial
- Samples currently being studied at Cavendish (along with additional QCL and optically pumped structures)
- New simulation for *n*-type SiGe recently developed
- *n*-type CVD growth due to start in Warwick this autumn