



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

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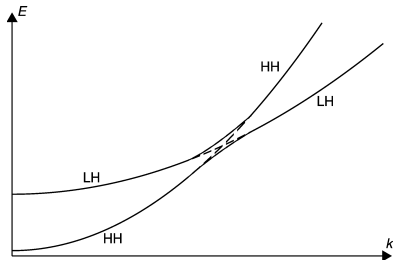


- 1 Si/SiGe QCLs
- 2 Pump–Probe Data
- 3 TEM Data
- 4 Ge Fraction due to Interdiffusion
- 5 Band Edge due to Interdiffusion
- 6 Implications for QCL Design

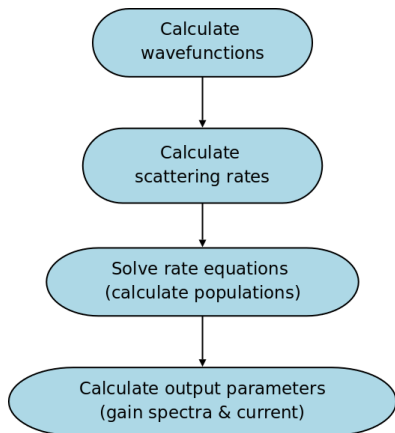


- In the modelling of heterostructures for intersubband lasers we generally assume abrupt interfaces
- Usually consider GaAs/AlGaAs
- Si/SiGe structures have much higher effective masses
- (So spatial extent of wavefunctions will be reduced)
- Dimensions of structures will therefore be smaller
- Ge more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

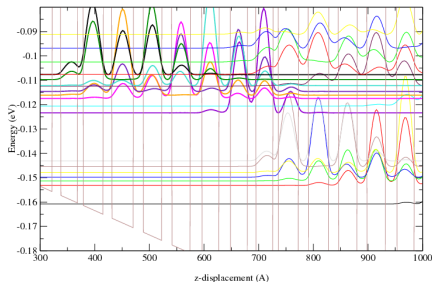
- $m^* = 0.49 m_0$  (HH)
- $m^* = 0.16 m_0$  (LH)
- Strain splits light- and heavy-hole states
- LH higher in energy (upside-down energy picture)
- Non-zero  $k$ -vectors, LH and HH mix
- QCL design philosophy: push light-hole states to higher energies



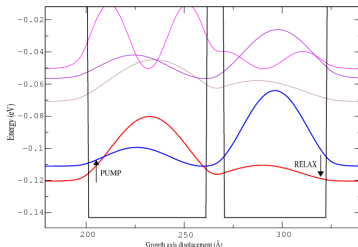
- 6x6 k.p bandstructure calculation
- Numerical solution of Schrödinger equation
- Scattering rates for: alloy disorder, interface roughness, carrier–carrier, ionised impurity, acoustic & optical phonons
- Assume Fermi distribution of carriers within subbands
- Solve rate equations self-consistently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



- 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?

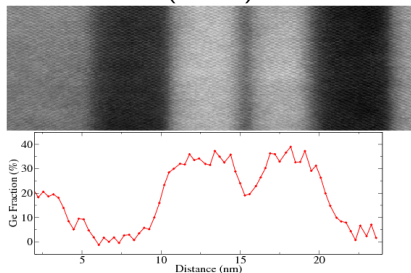


- 2 well structure grown for pump-probe measurements using the FELIX free electron laser facility at Utrecht
- $\text{Si}_{0.6}\text{Ge}_{0.4}$  wells, Si barriers.
- Measured dimensions for wells:  $61 \pm 0.6 \text{ \AA}$  and  $52 \pm 0.6 \text{ \AA}$ , with the barrier thickness  $8 \pm 0.6 \text{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

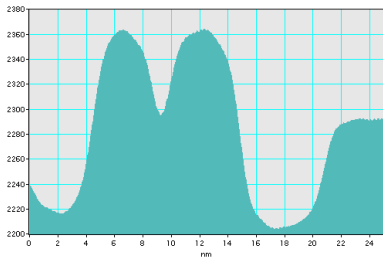


- aberration corrected superSTEM facility at Daresbury, UK. Data indicates interfaces may be diffuse
- EELS gives an intensity proportional to the atomic number
- Nominally pure Si barriers may actually contain significant Ge fraction
- Suggests interdiffusion of Si/SiGe may have significant effect on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

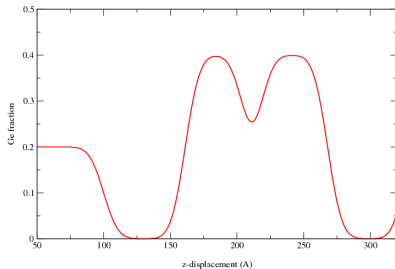
### Electron energy loss spectra (EELS)





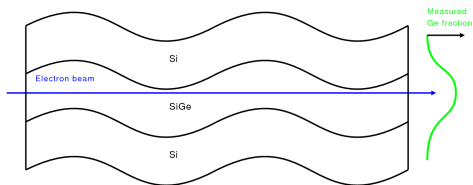


ADF profile



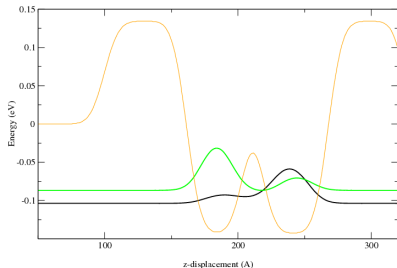
1.2 nm diffusion length,  
error-function interdiffusion

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



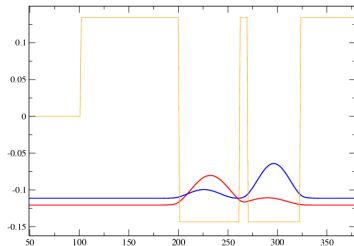


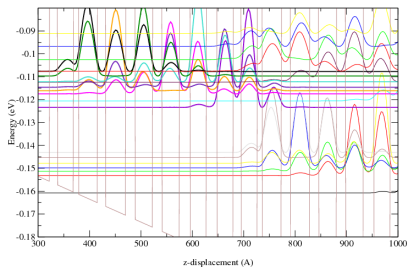
- 1 nm diffusion length
- Error function diffusion
- State separation = 15.4 meV (in agreement with pump-probe data)
- (Nominally pure) Si barrier now greatly reduced in energy



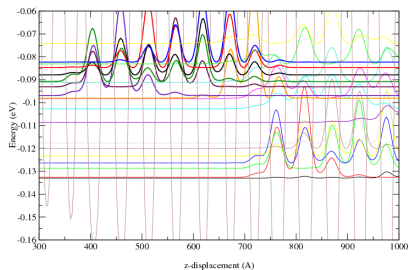


- Inclusion of the interdiffusion significantly alters band edge profile
- Wavefunctions change too
- Thin barriers become lower in energy
- In (low  $\mu$ ) SiGe systems, thin barriers are desired.





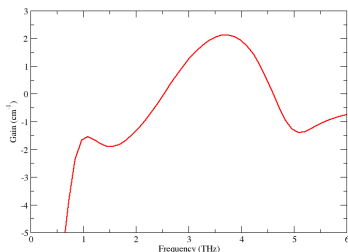
Existing *p*-type design



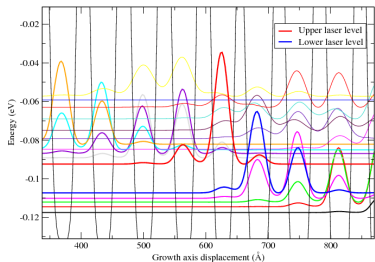
With interdiffusion

# Gain spectra

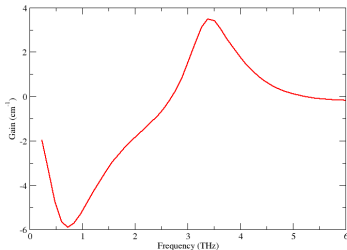
- Gain is lost for simulation with interdiffusion
- We just see a large broadband absorption
- Interdiffusion is clearly a significant design issue
- However, we can incorporate this into the design...



Gain spectra for original design



New design including  
interdiffusion



Simulated performance is similar  
to previous design



- 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