Conference or Workshop Item:
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Growth variation effects in two-dimensional Si/SiGe heterostructures

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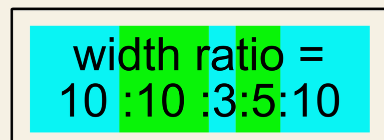
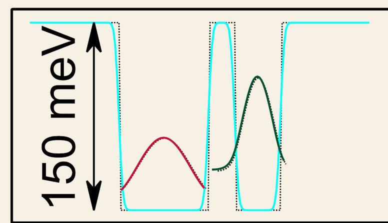
2D Si/SiGe heterostructures

- Potential candidates for photonic system-on-a-chip applications
- Resonant tunneling diodes have been demonstrated and electroluminescence observed from quantum cascade structures
- Most theoretical models assume abrupt interfaces but real interfaces may be diffuse
- Annealing leads to symmetric interdiffusion, with a diffusion length *L*. Similar results assumed for asymmetric surface segregation
- Potentially significant effects on band structure and carrier dynamics

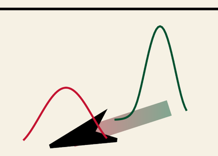
Theoretical approach



Specify structure: Pair of quantum wells (QW) [green=well, blue=barrier]



Simulate annealing and find band structure: 6×6 ***k.p*** model for *p*-type, 1-band effective mass for *n*-type.



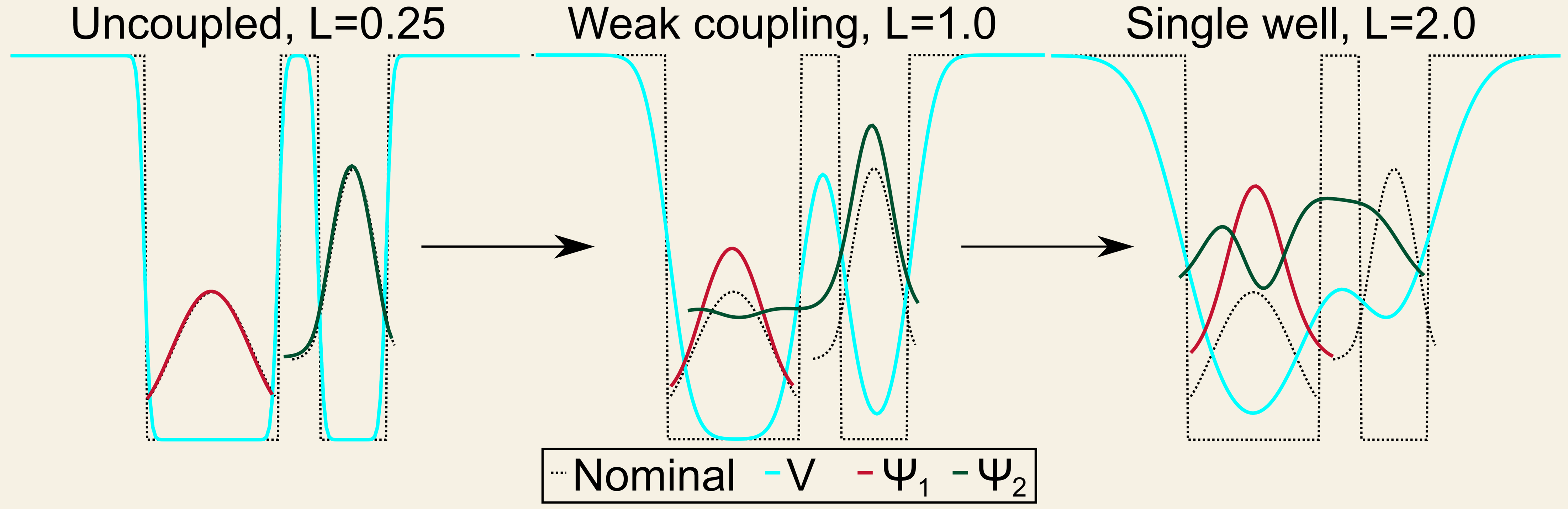
Time independent perturbation theory used to find average scattering rates from upper to lower subband.

Scattering processes

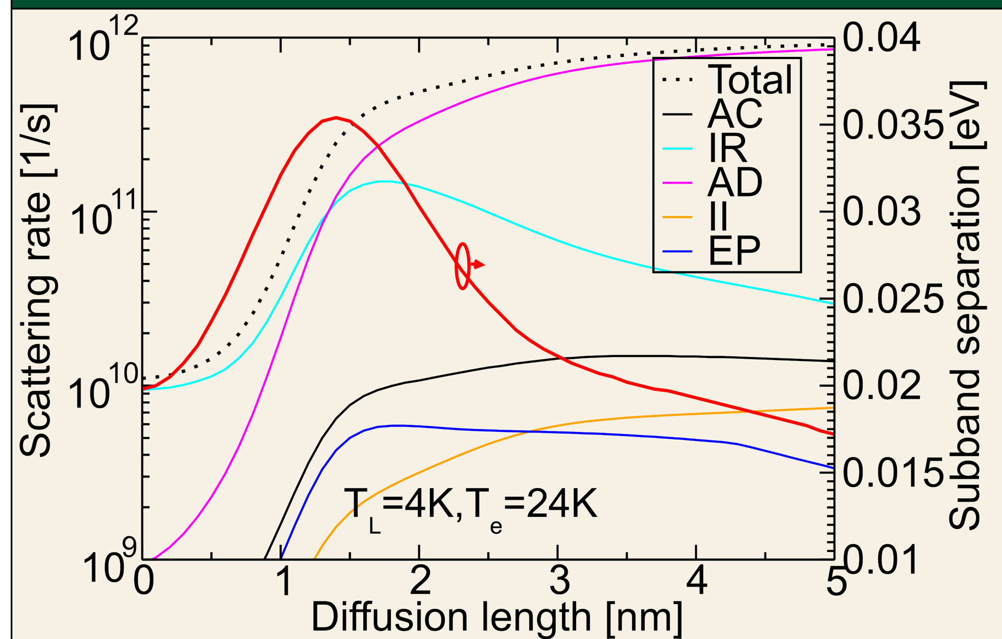
- Rapid alloy disorder (AD) scattering when wells contain mixture of Si and Ge
- Rapid interface roughness (IR) scattering when wavefunctions overlap interfaces
- Slow ionised impurity (II) and electron-electron (EE) scattering due to low doping
- Inelastic electron-phonon (EP) interactions increase with subband spacing ΔE and saturate when ΔE exceeds phonon energy
- All scattering processes, including elastic acoustic phonon (AC) scattering, increase with the overlap between wavefunctions

Effect on band structure

- Wavefunction overlap increases
- ΔE initially increases as wells narrow but decreases as wells merge



Simulated annealing calculations (*n*-type)

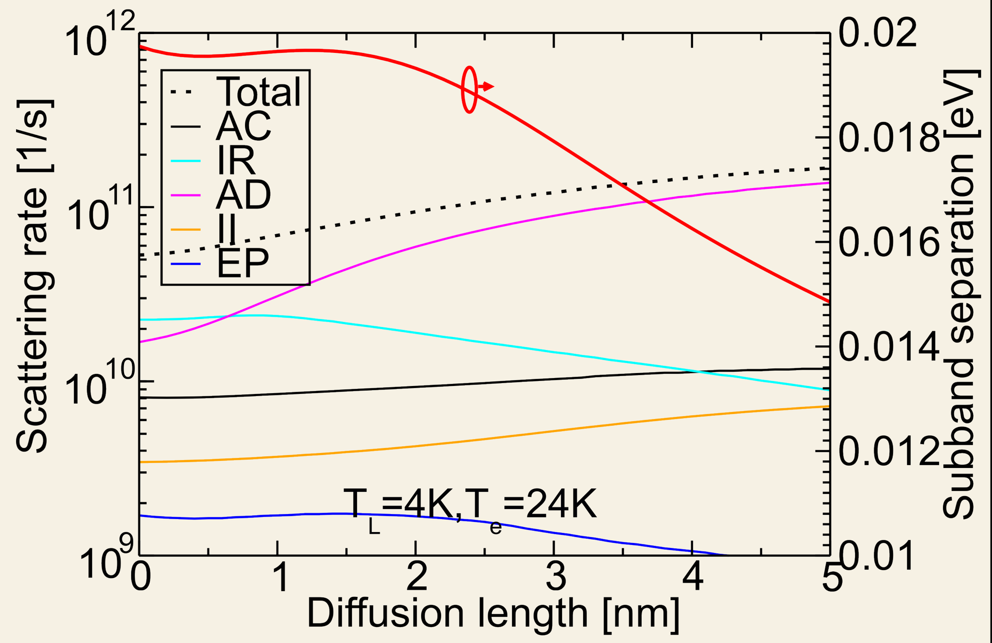


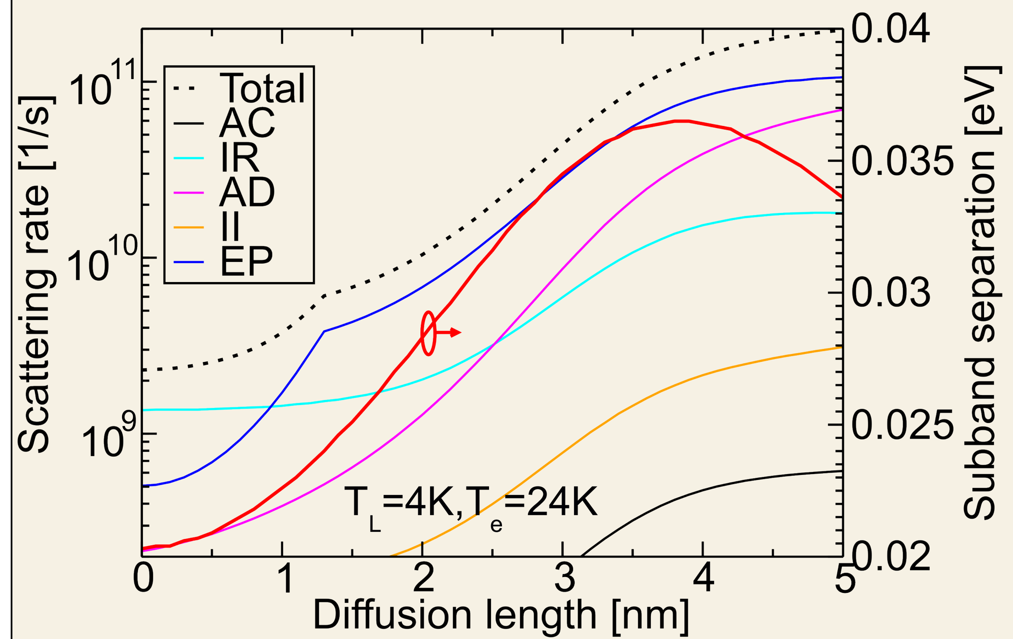
(001) oriented Si-rich systems

Large effective mass $m_q \approx 0.92 m_e \rightarrow$ thin layers. Widths vary rapidly with increasing *L* and ΔE is strongly affected. AD increases significantly due to Ge entering wells

(111) oriented Si-rich systems

$m_q \approx 0.26 m_e \rightarrow$ thicker layers are relatively insensitive to *L*. ΔE and scattering rates are therefore fairly stable. AD increase partly offset by IR decrease

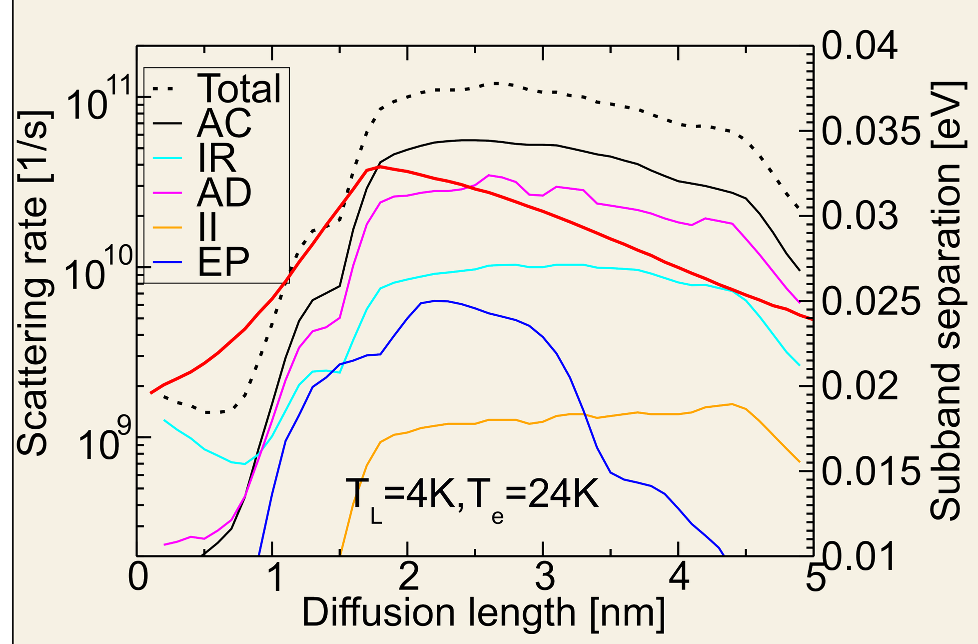




(001) oriented Ge-rich systems

$m_q \approx 0.12 m_e$. "single well" regime does not start until $L \sim 3.5$nm. Low phonon energy ($\hbar\omega$=28meV) leads to EP dominating when $\Delta E > \hbar\omega$. Other rates fairly stable in uncoupled regime.

Simulated annealing calculation (*p*-type)



(001) oriented Si-rich systems

Upper subband is light-hole ($m_q \approx 0.16 m_e$) when weakly coupled but heavy-hole ($m_q \approx 0.49 m_e$) otherwise. Large variation in mass strongly affects scattering rates.

Figures of merit

- Can define a set of figures of merit for tolerance to interdiffusion in the systems simulated in this work as follows:
  - L_{pk} – diffusion length resulting in maximal subband spacing. (Ideal value = ∞)
  - ΔE_{pk} – subband separation at first local maximum, relative to nominal value. (Ideal value = 1)
  - L_W – diffusion length yielding 50% shift in total intersubband scattering rate (Ideal value = ∞)

System	L_{pk} (nm)	ΔE_{pk}	L_W (nm)
n-type (001) Si-rich	1.41	1.75	1.27
n-type (111) Si-rich	1.37	0.99	1.49
n-type (001) Ge-rich	3.84	1.83	0.94
p-type (001) Si-rich	1.79	1.65	0.91

Conclusions

- Interdiffusion causes large changes in transition energies and scattering rates (particularly AD in *n*-type structures)
- Barrier degradation leads to merging of quantum wells.
- Transition energy shift in Ge rich systems increases electron-phonon scattering
- Scattering in *p*-type systems affected by change of upper subband from light-hole to heavy-hole character
- *n*-type (111) oriented Si-rich systems yield most stable transition energy and scattering rates due to low effective mass and high phonon energies