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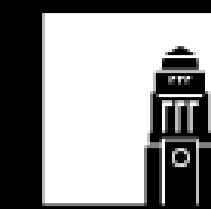
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# Growth variation effects in two-dimensional Si/SiGe heterostructures

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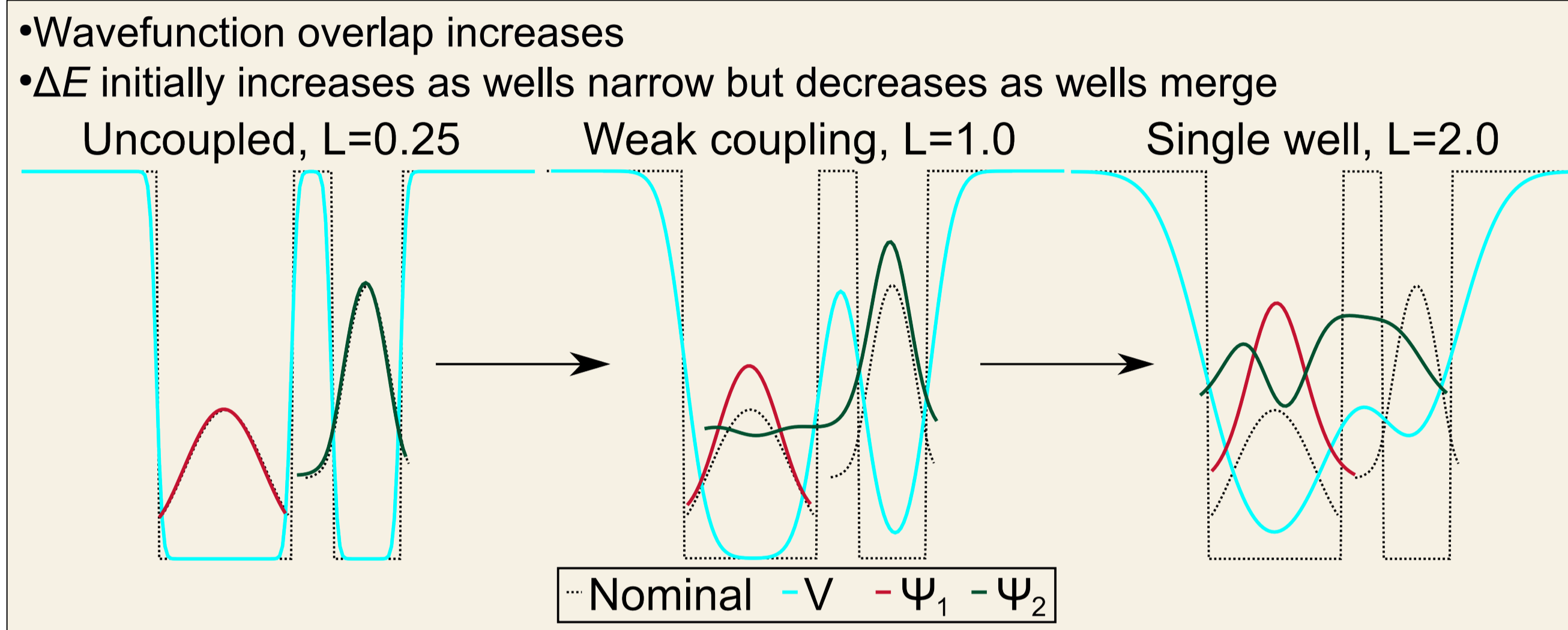


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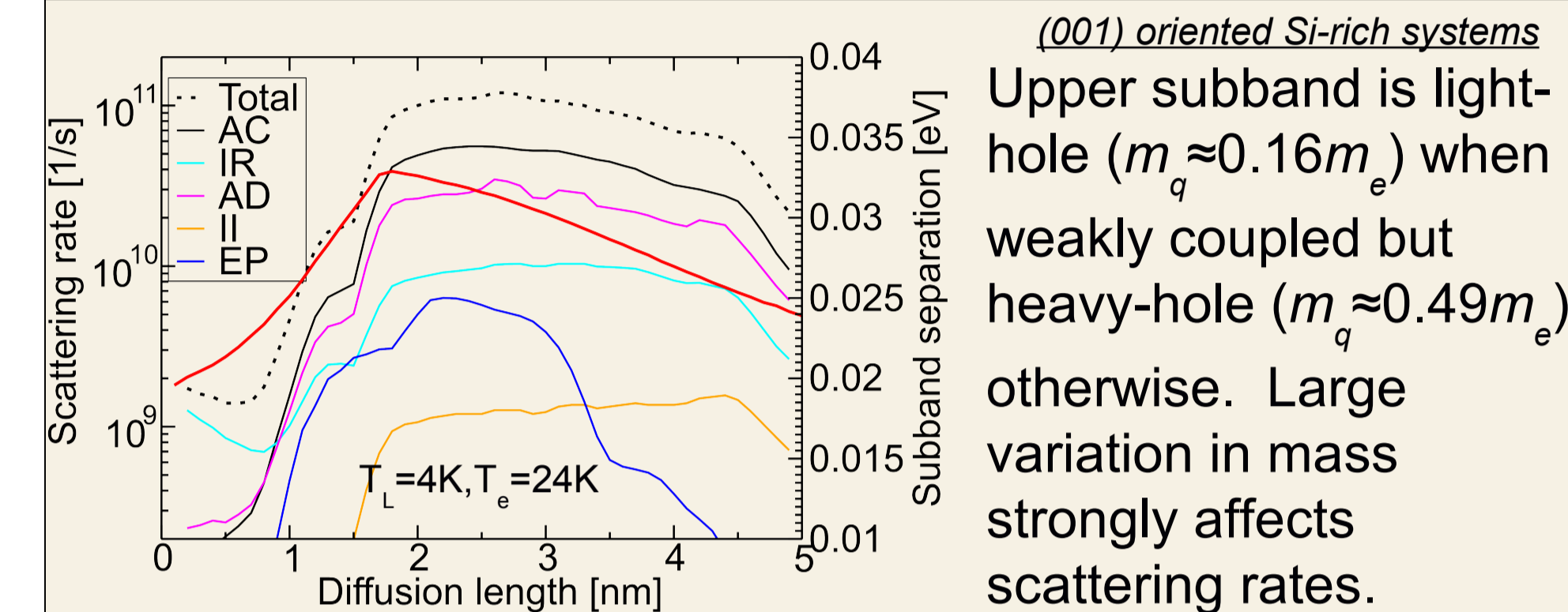
## 2D Si/SiGe heterostructures

- 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

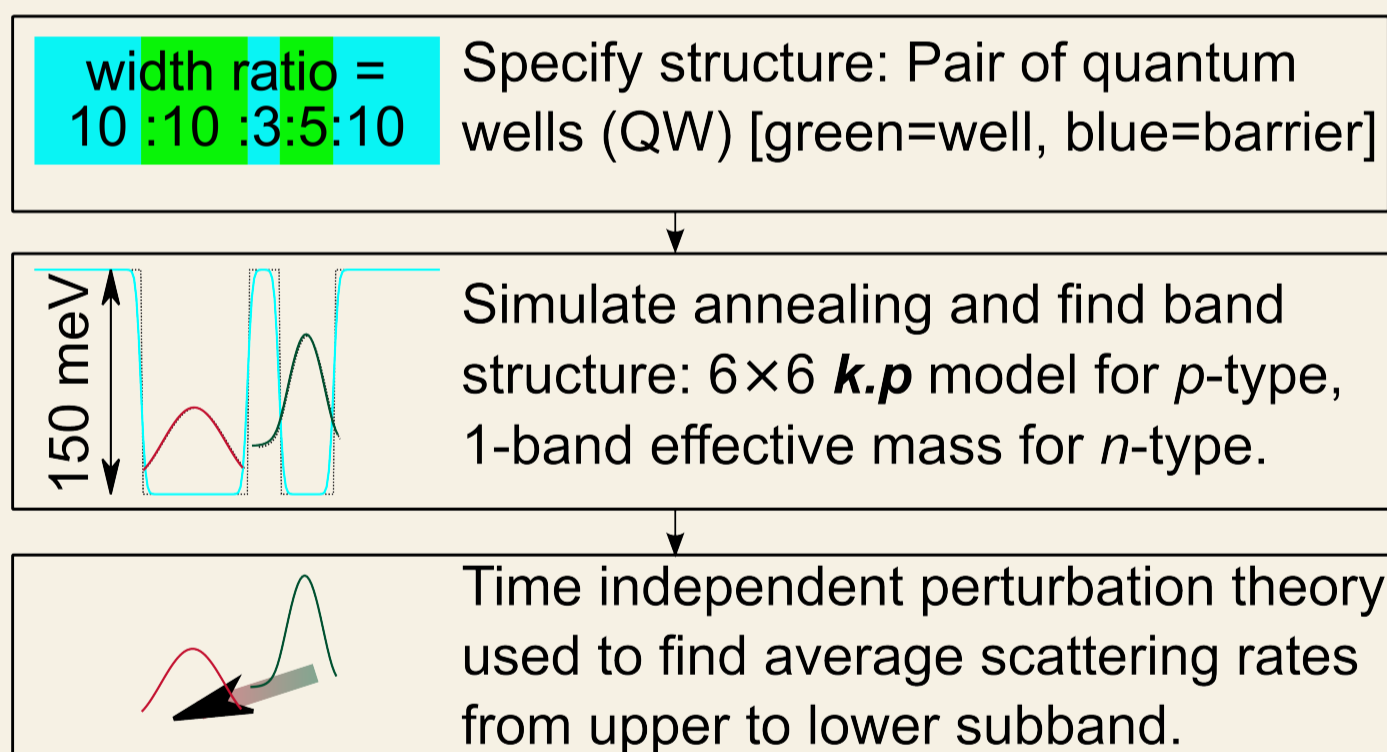
## Effect on band structure



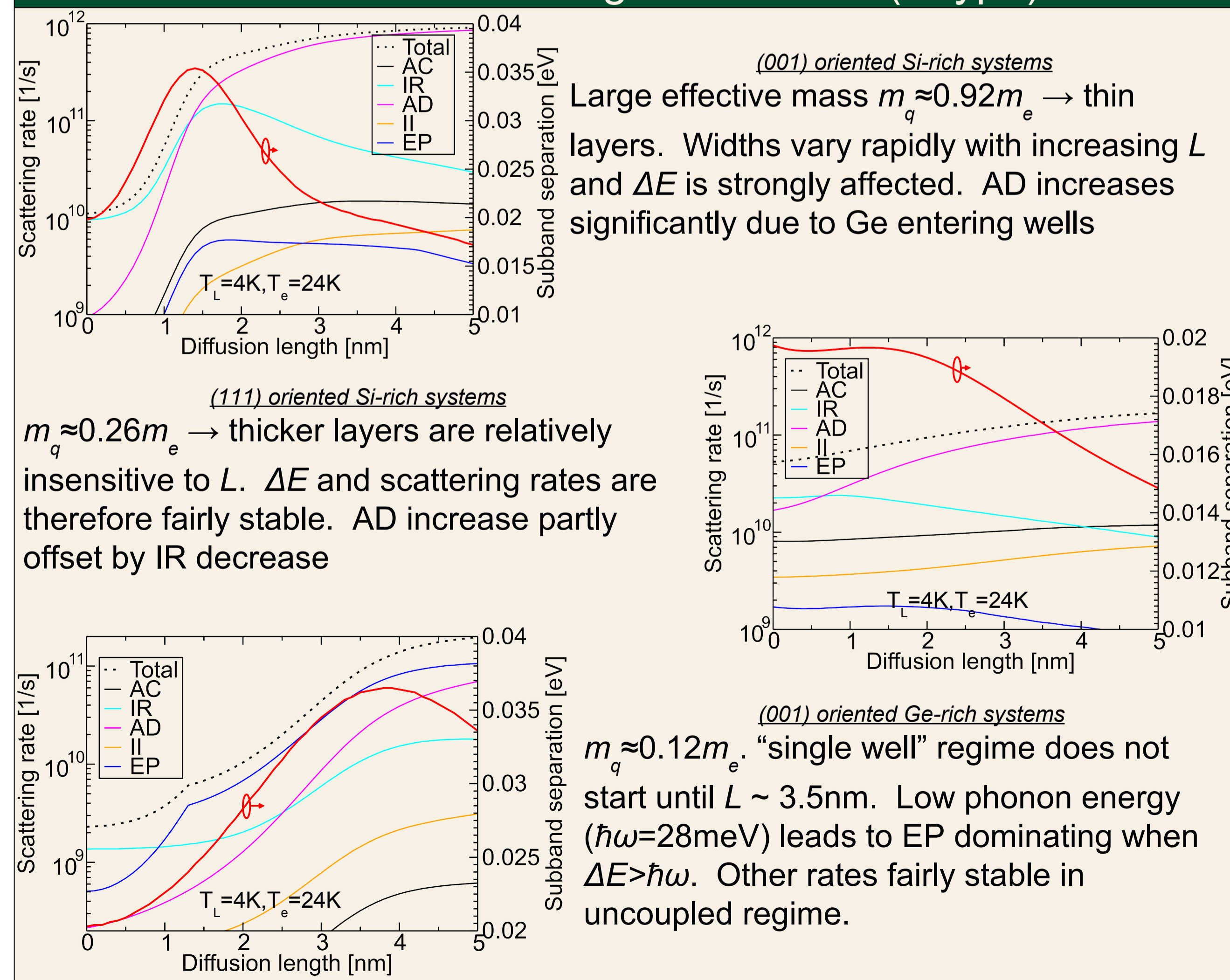
## Simulated annealing calculation ( $p$ -type)



## Theoretical approach



## Simulated annealing calculations ( $n$ -type)



## 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 =  $\infty$ )
  - $\Delta E_{pk}$  – 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 =  $\infty$ )

System	$L_{pk}$ (nm)	$\Delta E_{pk}$	$L_w$ (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

## 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  $\Delta E$  and saturate when  $\Delta E$  exceeds phonon energy
- All scattering processes, including elastic acoustic phonon (AC) scattering, increase with the overlap between wavefunctions

## 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