Intervalley mixing in two-dimensional n-type Si/SiGe heterostructures

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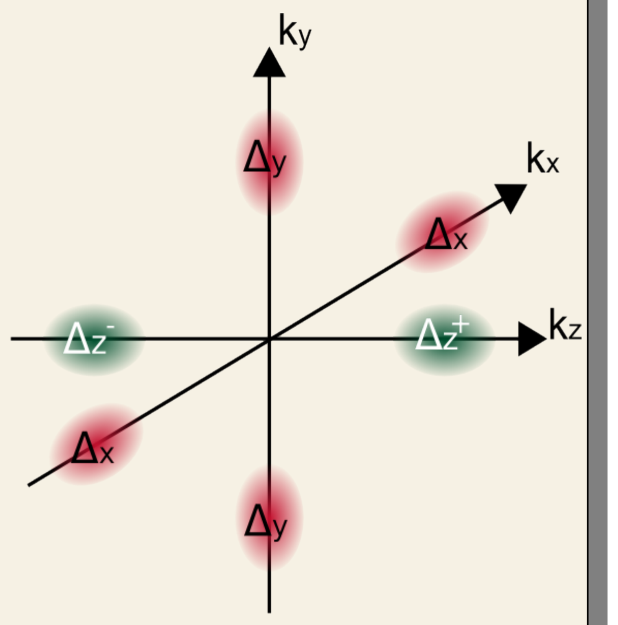
Si/SiGe conduction band

- Conduction band edge is located in the Δ valleys in k-space
- In a 2-dimensional heterostructure (*i.e.* free motion over *xy* plane), strain and effective mass anisotropy splits this degeneracy into two Δ_z and four $\Delta_{x,y}$ valleys



- Δ_z states have basis components with wave vectors centred around either Δ_z valley
- Mixing occurs between basis components reflected by interfaces normal to *z*-direction
- This mixing splits the degeneracy of Δ_z states

Effective mass approximation (EMA)

- Faster than atomistic methods *e.g.* empirical pseudopotential model (EPM)[1]
- *Usually* requires fitting parameters for valley splitting[2]
- Wave function for Δ_z states is weighted sum of basis components from each valley:

$$\Psi(z) = \left(a_1 e^{ik_0 z} + a_2 e^{-ik_0 z}\right)\varphi(z)$$

- For *symmetrical confining potentials*, the double valley EMA is self-contained.[3] Weighting coefficients are

$$a_{1,2} = \frac{1}{\sqrt{2}}(1, \pm 1)$$

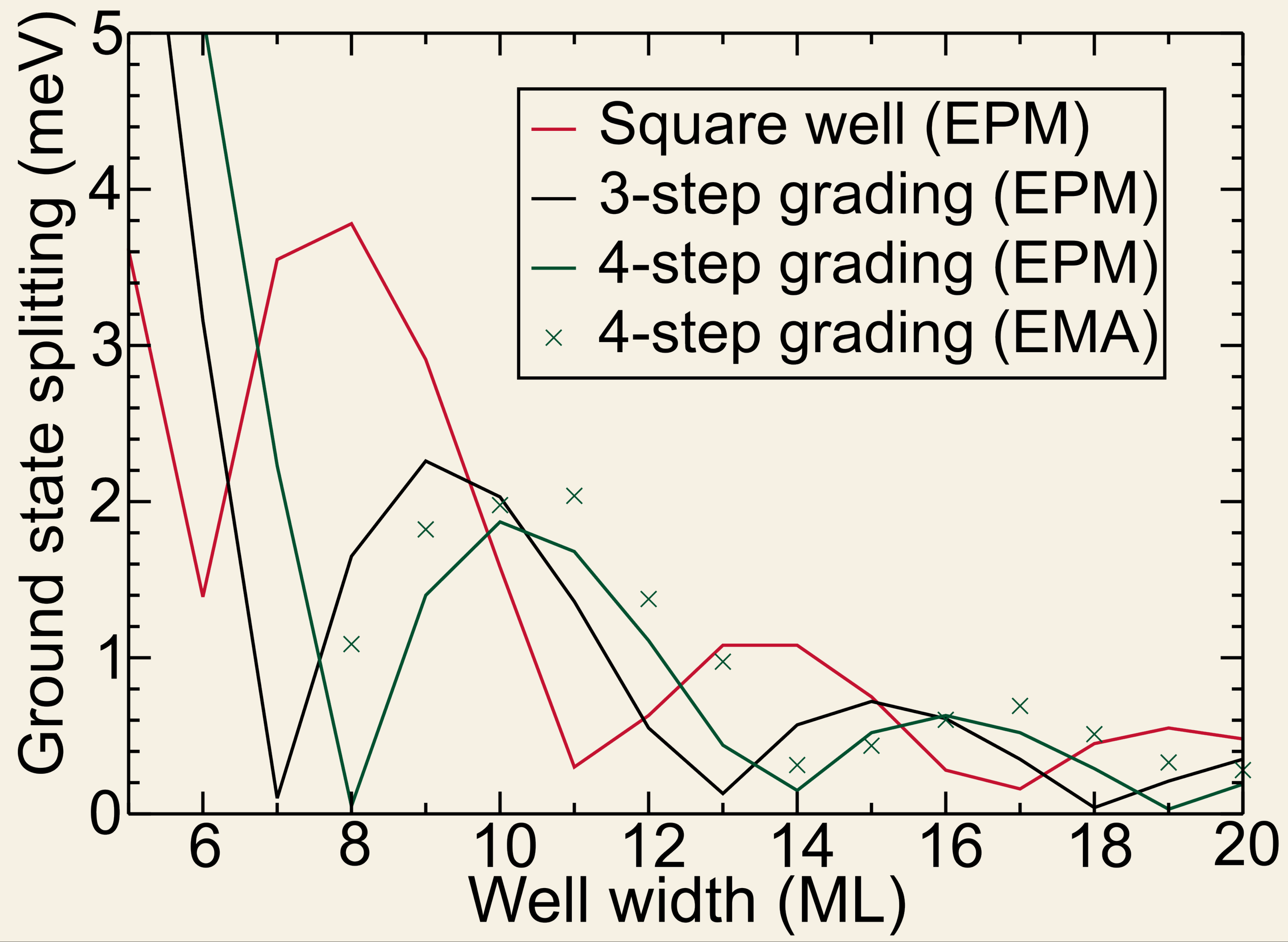
- A *splitting potential* term may be added to the effective mass Hamiltonian.
- It can be shown that this is a product of conduction band envelope potential and an oscillatory function of valley location:

$$U(z) = \pm V(z)\cos(2k_0 z)$$

- We have shown that even for slightly asymmetrical structures, the DVEMA agrees well with the EPM.[4]

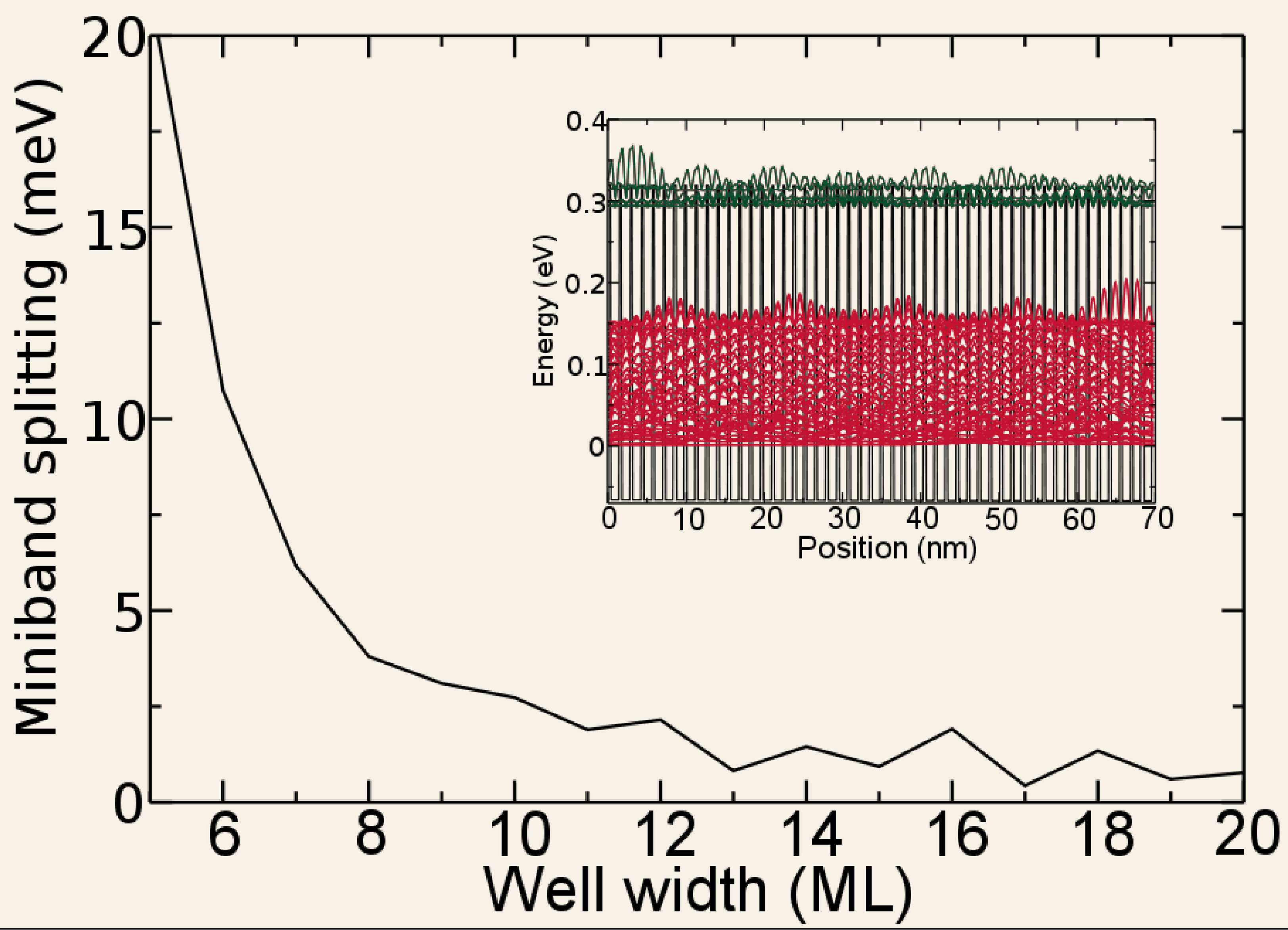
Diffuse interfaces

- Valley splitting is a decreasing, oscillatory function of well width.
- Plot shows splitting in quantum well (QW) with Si wells and $Si_{0.5}Ge_{0.5}$ barriers on $Si_{0.8}Ge_{0.2}$ substrate
- 1ML = half lattice constant
- Ge diffusion modelled for 3 to 4 ML diffusion length
- Diffuse interfaces are modelled as piecewise linear gradings in atomistic simulations
- EMA results agree with EPM (sample data in plot)
- Splitting decreases as interfaces are smoothed



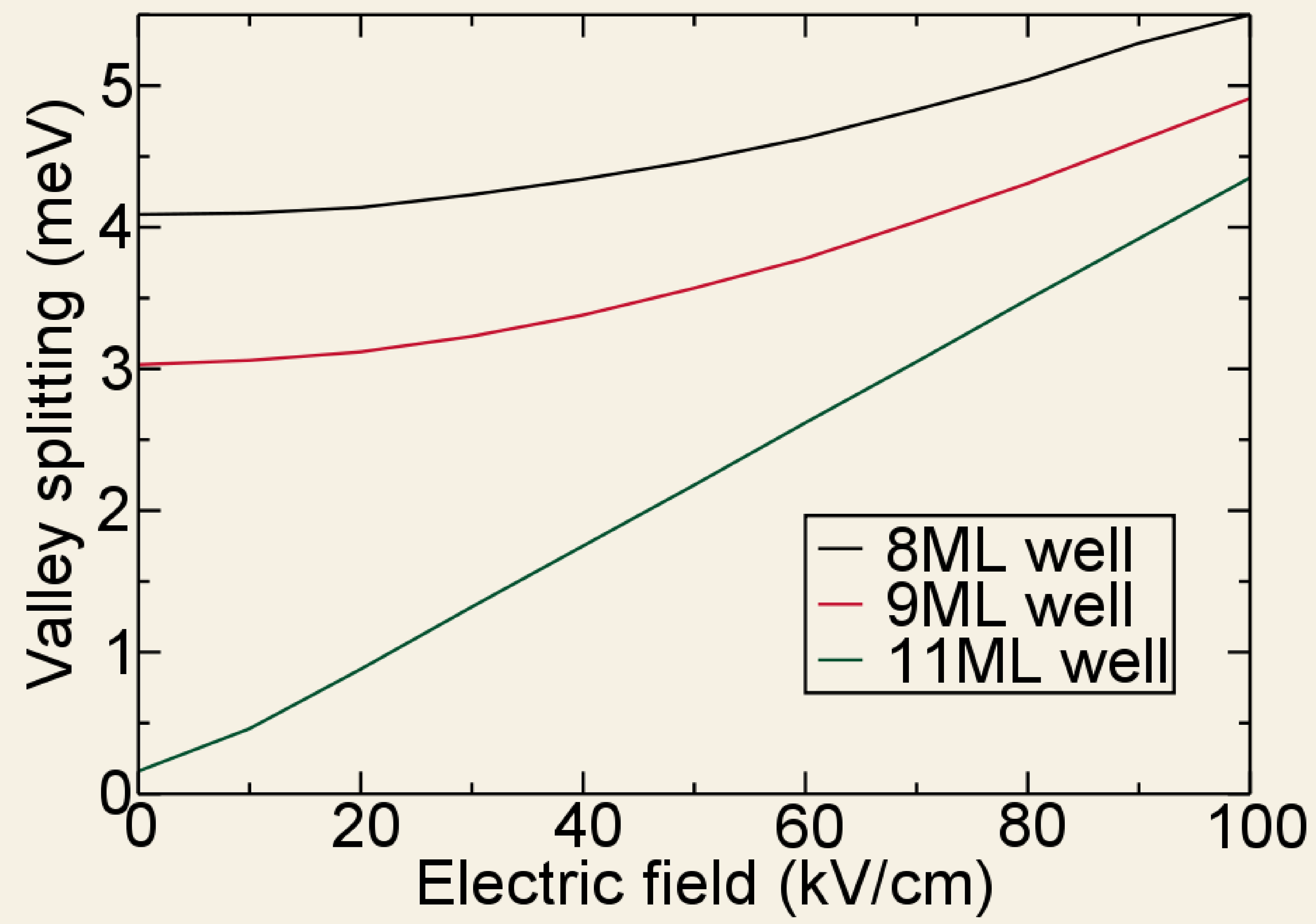
Quantum cascade lasers (QCL)

- Graph below shows EPM model of valley splitting in lowest pair of Si/SiGe superlattice (SL) minibands as function of well width.
- Constant 4ML, $Si_{0.5}Ge_{0.5}$ barrier and variable width Si well on $Si_{0.8}Ge_{0.2}$ substrate. Well widths up to around 5.4nm are simulated.
- Inset shows that the miniband in a SL approximates a "miniband" in a QCL. 50 periods of the envelope potential were used to generate the plotted EMA Schrödinger solution.
- SL splitting decreases rapidly with well width
- Oscillations are smaller than QW plot above, but magnitude is larger overall
- In QCLs, "miniband" states are not continuous, but are actually closely spaced discrete states.
- QCL solution is computationally demanding but is located between the SL and QW cases.



Electric field

- Applied electric field weakens confinement on one side of well
- Splitting is independent of well width at high fields



Conclusions

- Splitting is decreasing, oscillatory function of QW width at low electric field
- EMA works well in symmetric structures
- Increases at high electric field and is independent of width
- Splitting also decreases with well width in unbiased SLs
- Very low splitting in wide, unbiased QWs such as those in optically pumped lasers
- Significant effect in strongly biased narrow QWs and narrow well SLs. May affect n-type Si/SiGe QCLs

Related publications

[1] Z. Ikonić, R. W. Kelsall and P. Harrison, Phys. Rev. B **64**, 125308 (2001).
[2] M. Friesen, S. Chutia, C. Tahan and S. N. Coppersmith, Phys. Rev. B. **75**, 115318 (2007).
[3] D. Z.-Y. Ting and Y.-C. Chang, Phys. Rev. B **38**, 3414 (1988).
[4] A. Valavanis, Z. Ikonić and R. W. Kelsall, Phys. Rev. B **75**, 205332 (2007).