

Valley degeneracies in (111) Si quantum wells

Objective

- Resolve discrepancies in experimentally observed and theoretically predicted valley degeneracies
- Study effect of surface morphology on the electronic structure

Approach

- Supercell tight-binding calculations to model surface miscuts
- Effective mass based valley-projection model to determine the directions of valley-minima of large supercells

Impact

- Atomistic basis representation is essential to capture the effect of mono-atomic steps on the electronic structure
- Surface miscut of (111) Si is found to be the origin of breaking of 6 fold valley degeneracy into lower 2 fold and higher 4 fold valley degeneracies

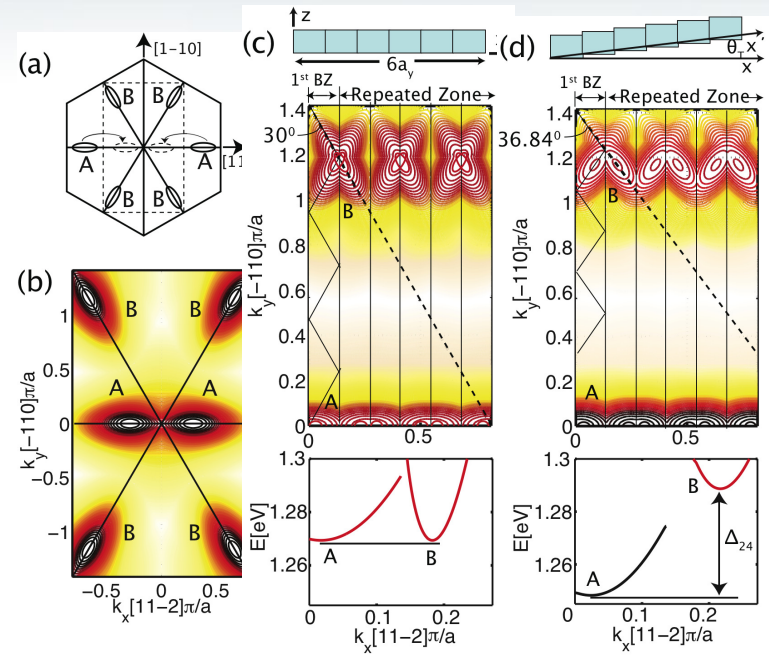


Fig: Origin of 2-4 splitting in miscut (111) Si QWs

Results

- Flat (111) Si QW shows 6 fold valley degeneracy
- Miscut causes 2-4 splitting due to different effective masses in confinement direction