Valley Degeneracy in (110) Si Quantum Wells: Strain and Misorientation Effects

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INTRODUCTION

Si-based devices are being pursued for quantum computing and spintronics due to their scaling potential and integrability within the present industrial nanoelectronic infrastructure. Relative energies and degeneracies of valley states are critical for device operation in these novel computing architectures and conventional MOSFET devices at nanometer scale. Bulk Si has six equivalent conduction band minima. In (110) Si quantum wells (QWs), this degeneracy is reduced to 4 fold in effective mass approximation (EMA) [1]. However, experimental results show ground state degeneracy factors of both 2 and 4 [2-4].

Similar inconsistencies between experimentally measured and theoretically predicted valley degeneracies are observed in (100) and (111) Si QWs [4,6,7]. Earlier work has shown that these inconsistencies are attributed to the presence of surface miscuts, which can be explicitly modeled in an atomistic method [6,7].

This work employs the tight-binding method to investigate the valley degeneracy of (110) Si QWs. Two mechanisms, (i) different confinement effective mass and (ii) valley-valley interaction are identified as the main degeneracy breaking mechanisms. Surface miscut is found to explain the experimentally observed valley degeneracy factors of 2 and 4.

APPROACH

A rectangular unit cell is used which is also primitive cell for (110) QWs. Implementation of rectangular cell provides a twofold advantage [5]. First, rectangular geometry simplifies underlying mathematics and implementation of periodic boundary conditions in the bandstructure calculation. Second, surface miscut can be easily implemented by applying shifted boundary condition to the rectangular supercell Fig 1(b).

The valence-force-field method with Keating potential is used for strain relaxation and $sp^3d^5s^*$ tight-binding method is used for calculating electronic structure. Calculations are performed using the general purpose electronic structure simulator, NEMO-3D [8, 9].

RESULTS AND DISCUSSION

A 5nm thick flat QW is first simulated. The 6-fold bulk degeneracy is lifted to a lower 4-fold and higher 2-fold valleys due to different confinement effective mass (Δ42 in Fig. 2) [6, 11]. The lower 4-fold degeneracy is further lifted by valley-valley interaction (Δ4 in Fig. 2(a)) [7,10]. This valley-valley interaction gives rise to the reported 2-fold degeneracy for ground state [3,4].

Experimentally observed 4-fold degeneracy can occur when quantum well is grown on a miscut surface. As an example, a 5 degree miscut tilted towards (111) direction is considered. Valley-valley interaction in this structure is suppressed and degeneracy factor 4 is recovered (Fig. 3) [3,11].

More realistic structures are subject to electric fields due to gate voltages or modulation doping as well as strain due to growth on SiGe substrates. Electric fields as well as strain are known to modulate the valley splitting [7,10]. Here we consider 25nm thick Si slabs subject to a variety of electric fields and strains.

CONCLUSION

Two degeneracy breaking mechanisms are identified in Si QWs: different confinement effective mass and valley-valley interaction. Strain and electric field are found to enhance both types of

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valley splitting. Wafer miscuts towards (111) give rise to different valley degeneracy factors from flat wells and explain experimentally observed inconsistency.

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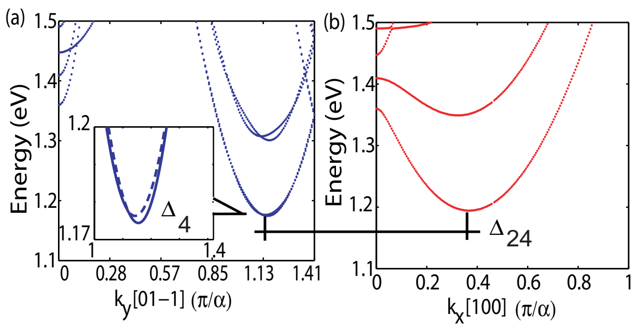

Fig. 2. Bandstrcture for flat Si (110) QWs. (a) Bandstructure along symmetric direction [01-1]. Insert shows the lowest two bands and presents VS due to valley-valley interaction, which results in two pairs of valleys slightly shifted in energy. (b) Bandstructure along symmetric direction [100]. Two figures are plotted with same energy scale to show VS due to different confined effective masses.

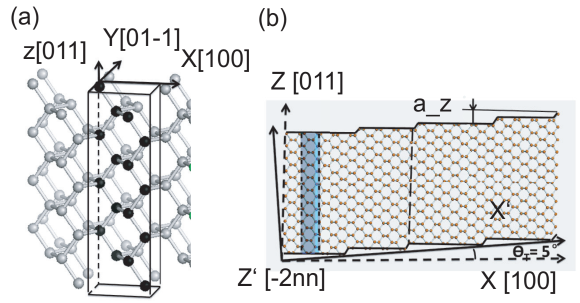

Fig. 1. Atomistic schematics of unit cells. (a) Rectangular unit cell of flat QW. (b) Unit cell of a 5 degree miscut (110) Si QW with monolayer steps. Interface mono-atomic steps are assumed to run parallel to (100) direction.

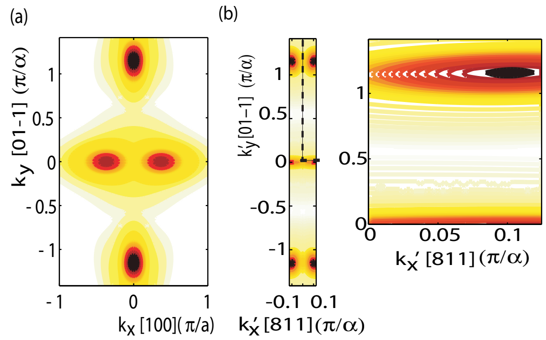

Fig. 3. 2D contour plot for lowest band of Si (110) quantum well. (a) Flat Si (110) quantum well. (b) 5 degree tilted Si (110) quantum well. Brillouin zone is roughly one eighth of bulk Si in kx direction due to supercell calculation. (right) Zoom in dashed area in left figure, only showing one quadrant of Brillouin zone. Positions of valley minima could be estimated by a valley projection model [11]. Strong interaction occurs at higher energies creating a minigap, which will be irrelevant to device operation.

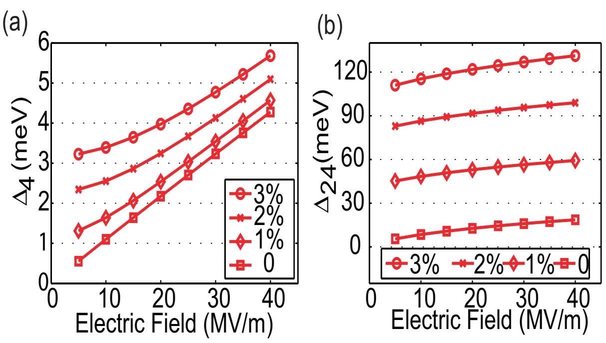

Fig. 4. Effects of strain and electric field on valley splitting in 25 nm Si (110) QWs. (a) Δ_4 type valley splitting of QWs with biaxial tensile strain in the presence of electric field. 3% strain corresponds to a Ge composition of 81%. (b) Behaviors of Δ_{24} type valley splitting with same strain and electric fields in (a).