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Valley-splitting in strained Silicon quantum wells on a miscut substrate using tight-binding model. NEERAV KHARCHE, MARTA PRADA, School of Electrical and Computer Engineering, Network for Computational Nanotechnology, Purdue University, TIMOTHY BOYKIN, Department of Electrical and Computer Engineering, University of Alabama in Huntsville, GERHARD KLIMECK, School of Electrical and Computer Engineering, Network for Computational Nanotechnology, Purdue University — The splitting of the two-fold degeneracy of conduction-band valleys in bi-axially strained SiGe/Si/SiGe quantum wells (QWs) grown on (001) and 2^o miscut substrates is computed as a function of magnetic field using semi-empirical nearest-neighbour $sp^3d^5s^*$ tight-binding model in NEMO-3D. Unlike flat QWs, miscut QWs show two degenerate valleys centred at $(k_x, k_y) = (\pm k_x^0, 0)$. Interaction between these two valleys due to confinement in the lateral (perpendicular to growth) dimension, leads to valley splitting (VS) in miscut quantum wells. VS in miscut QWs is suppressed by at least two orders of magnitude as compared to flat QWs. Numerical calculations with perfect step ordering underestimate experimentally observed VS. Simulation of experimental non-idealities such as step-roughness and alloy-disorder raise computed VS to the experimentally observed values.

Neerav Kharche
School of Electrical and Computer Engineering, Network for
Computational Nanotechnology, Purdue University

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