Optical Properties of Single Nanometer-Thick Quantum Wells of Crystalline Silicon

D.J. Lockwood[1] and Z.H. Lu[2]

[1]Institute for Microstructural Sciences, National Research Council, Ottawa, Ontario K1A 0R6, Canada
[2]Department of Materials Science and Engineering, University of Toronto, Toronto, Ontario M5S 3E4, Canada

Single nanometer-thick layers of crystalline silicon (c-Si) confined by amorphous SiO_2 have been prepared by chemical and thermal processing of ELTRAN silicon-on-insulator wafers. The quantum wells of c-Si thus formed have sharp interfaces and exhibit a marked band gap increase with decreasing layer thickness, d, for d < 3 nm [1]. The room-temperature photoluminescence (PL) from these ultra-thin single wells can be resolved into two bands (see Fig. 1). One band exhibits a strong increase in peak energy with decreasing d, while the other band remains nearly constant in energy at about 1.8 eV (see Fig. 2). The band gap energy variation predicted from theoretical calculations based on self-consistent full potential linear muffin-tin orbital [2] and first-principles projector-augmented wave [3] methods are also shown in Fig. 2. Comparison with theory shows that the increase in PL peak energy is precisely that predicted for the c-Si energy gap, confirming that this PL band is due to quantum confinement of carriers in the c-Si well. The other PL band is attributed to recombination of confined electron-hole pairs at the c-Si/SiO_2 interface rather than within the quantum well, similar to what has been observed previously in oxidized silicon nanocrystals [3].

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