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

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The discovery by Lu et al. [1] of intense luminescence in Si/SiO_2 superlattices grown by molecular beam epitaxy has led to numerous experimental and theoretical studies of their structural, electronic and optical properties. A blue shift of the optical properties with increased quantum confinement is reported in most experimental and in all theoretical studies. In general, the atomic structure of Si in these quantum wells is amorphous, as is also the case for the two SiO_2 barriers. This is due to the growth process in combination with the considerable lattice mismatch between Si and SiO_2 in their crystalline phases. Recently, single nanometer-thick layers of crystalline Si (c-Si) confined by amorphous SiO_2 have been prepared by chemical and thermal processing of Canon epitaxial layer transfer (ELTRAN) silicon-on-insulator wafers. The quantum wells of c-Si thus formed have very sharp interfaces and exhibit a marked band gap increase with decreasing layer thickness, d, for $d < 3$ nm [2].

The room-temperature photoluminescence (PL) from these ultra-thin crystalline single wells has been measured and it 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 [3] and first-principles projector-augmented wave [4] 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 [5].

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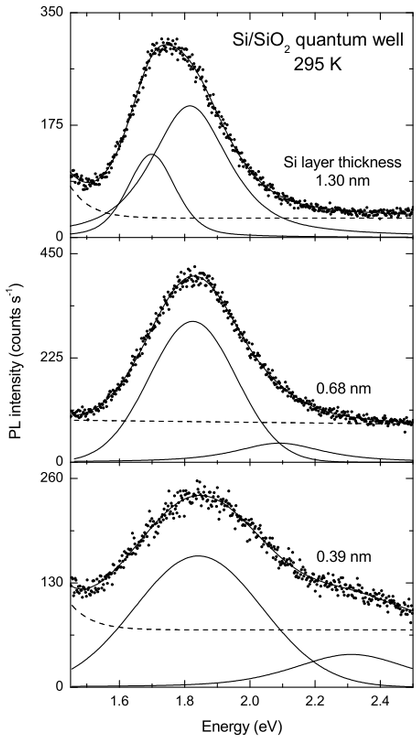

Fig. 1. Room temperature PL from single c-Si/SiO_2 quantum wells of different thicknesses. The PL line shape has been fitted with the two bands (indicated by the solid line passing through the data points) shown below by the solid lines. The dashed line is the fitted background.

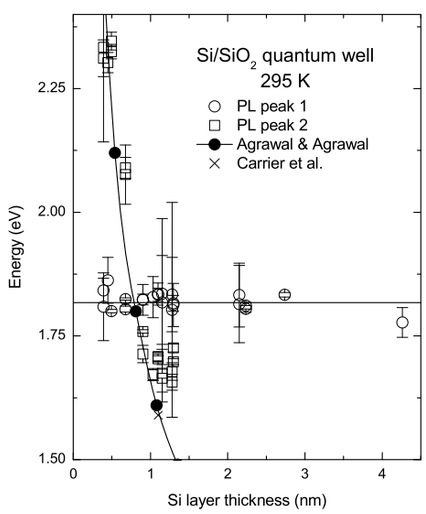

Fig. 2. Experimental results (O,□) for the energies of the two PL bands of c-Si/SiO_2 quantum wells as a function of well thickness compared with the theory of Agrawal and Agrawal (◊) [2] and Carrier et al. (X) [3]. (The solid line is an interpolation of the theoretical data.) The error bars represent the standard deviation in the peak energy determined from the fits. The horizontal solid line is a least squares fit to the data of peak number 1.