# Quantum confinement effects in strained silicon-germanium alloy quantum wells

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We report the first detailed study of quantum confinement shifts of band-edge photoluminescence energies in Si/strained $Si_{1-x}Ge_x$/Si single quantum wells. A quantum confinement energy of up to 45 meV has been observed for quantum wells as small as 33 Å in width. The experimental results are in good agreement with a calculation of the hole confinement energies. The hole energy levels in quantum wells were obtained by numerically solving effective-mass equations with proper matching boundary conditions at interfaces using a $6 \times 6$ Luttinger–Kohn Hamiltonian. Both strain and spin-orbit interactions were included in the calculation.

In recent years, the $Si/Si_{1-x}Ge_x$ strained layer system has attracted an enormous amount of attention because of its potential applications in silicon-based high-speed electronic circuits as well as in new optoelectronic devices. Even though many novel devices such as heterojunction bipolar transistors (HBTs),[1] resonant tunneling diodes (RTDs),[2] and high mobility two-dimensional-hole gases[3] have been successfully demonstrated in the $Si/Si_{1-x}Ge_x$ strained layer system, many fundamental parameters are still being sought after, among them the hole effective masses of the strained $Si_{1-x}Ge_x$ alloys. In this letter we report the first direct measurement of the exciton energies of such strained $Si_{1-x}Ge_x$ quantum wells through band-edge photoluminescence. The results are then shown to be in good agreement with hole ground state energies obtained from an exact solution of the effective-mass equations using a full $6 \times 6$ Luttinger–Kohn Hamiltonian.

The structures used in the experiment are $Si/Si_{0.8}Ge_{0.2}$/Si quantum wells grown by rapid thermal chemical vapor deposition (RTCVD)[4] on 100 mm (100) silicon substrates. The silicon layers were grown at 700 °C from dichlorosilane, and the silicon germanium layers at 625 °C.[5] Further growth details can be found in Ref. 4. The $Si_{0.8}Ge_{0.2}$ layers were fully strained with a misfit dislocation spacing of greater than 1 mm. The thickness of the wells ranged from 33 to 83 Å. Quantum well thickness was confirmed on several samples (33, 45, and 67 Å) by direct inspection by cross-section transmission electron microscopy (TEM), and also independently by Rutherford backscattering spectroscopy (RBS). Assuming $Si_{1-x}Ge_x$ composition of $x = 0.20 \pm 0.02$ (from x-ray diffraction measurement on thicker samples), that the composition was not a function of growth time, and abrupt interfaces, the $Si_{1-x}Ge_x$ thickness can be easily calculated from the total 2-D Ge density measured by RBS. Two methods yielded the same thickness within 4%. From TEM (Fig. 1) and also from Auger electron microscopy profiling, the transition width at the interfaces was found to be 10 Å or less. On samples not measured as described above, the well widths were estimated by comparing the growth times to those of the above samples. The silicon cap layers were $\sim 160$ Å thick for all samples. The photoluminescence (PL) spectra were taken using green light excitation from an argon-ion laser. 4 and 77 K spectra were taken with samples immersed in a liquid helium and liquid nitrogen bath, respectively.

The PL spectra of several of our samples with well widths ranging from 33 to 83 Å are shown in Fig. 2 for 4 and 77 K. Photoluminescence in $Si_{1-x}Ge_x$/Si structures has been observed from unknown sources with an energy well below the band gap,[6] band-edge excitons,[7,8] and in "zone-folded" Si/Ge superlattices,[9,10] although the "zone-folded" PL may be due to dislocations[11] and not to the superlattice itself. By comparison to previous results in strained $Si_{1-x}Ge_x$ alloys,[7] the features in the spectra of Fig. 2 may immediately be identified as band-edge exciton luminescence.

The highest-energy peaks in the 4 K spectra represent no-phonon (NP) recombination of bound excitons primarily due to alloy randomness.[12] At higher temperatures, such as 77 K, the NP PL is from free excitons at low power
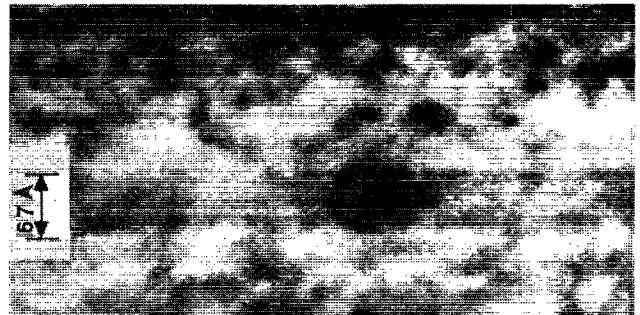


FIG. 1. High resolution cross-section TEM of a $Si/Si_{0.8}Ge_{0.2}$/Si sample with a quantum well width of 67 Å.
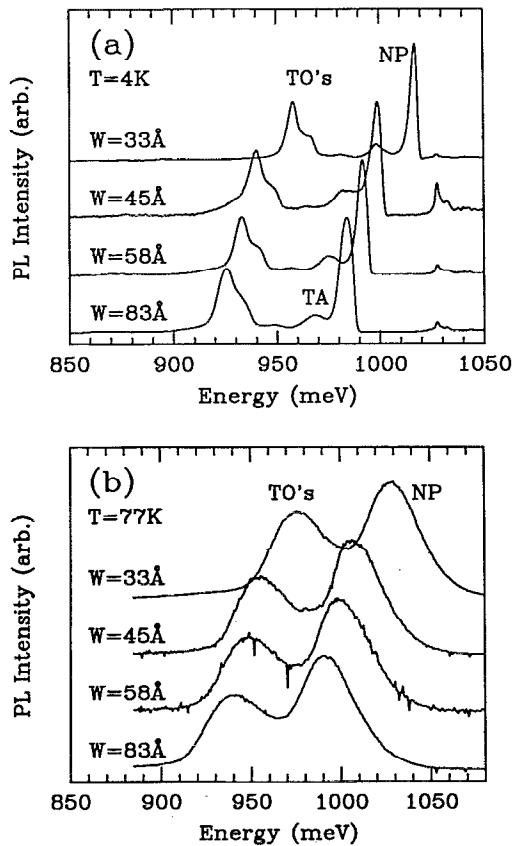
FIG. 2. Photoluminescence spectra of four $Si/Si_{0.8}Ge_{0.2}/Si$ quantum well samples with thickness of 33, 45, 58, and 83 Å at (a) 4 K and (b) 77 K.
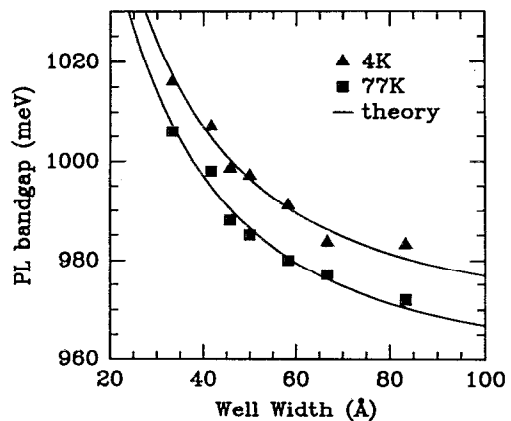


FIG. 3. PL band gap vs quantum well width at 4 and 77 K. The solid line is from the exact subband calculation. The bulk band gap was fit independently at each temperature and the dashed line. The error bars on the data points are ±2 meV and ±5 Å.

densities,[7] and electron-hole plasmas (EHP) at high power densities.[13] Because no phonons are involved, the NP signal is an accurate measure of the band gap except for exciton binding energies at 4 K and renormalization effects due to the high-carrier densities in the plasmas at 77 K (about 10–20 meV). This NP signal will be used in this letter to track the exciton energy in the quantum well. The lower-lying signals at both 4 and 77 K are phonon replicas, of which the transverse optical is the most prominent.[7,12]

As the quantum well thickness is reduced, one notes a monotonic shift in the PL band gap to larger values. This is expected because of the effect of quantum confinement on the energy levels in the well. To the best knowledge of the authors, this is the first time this shift has been directly observed in the $Si/Si_{1-x}Ge_x$ system. The photoluminescence band gaps extracted at 4 and 77 K[13] are shown versus well width in Fig. 3. The 77 K PL band gaps are consistently lower than the 4 K PL band gaps, presumably due to the band-gap reduction at the higher temperature and due to differences between the exciton binding energies and renormalization energies mentioned above. The relative shift of the band gaps with well width is similar at both temperatures, however.

The band-gap offset in the $Si$/strained $Si_{1-x}Ge_x$ system for low $x$ values is known to be predominantly in the valence band.[14,15] For $Si_{0.8}Ge_{0.2}$, the conduction band offset has been calculated by Van de Walle[15] to be less than $\sim 20$ meV, while the valence band offset is much higher ($\sim 160$

meV). Therefore we have focussed on the valence band and neglected the confinement effect in the conduction band in our calculations. Also neglected was any possible variation of exciton binding energy with well width. The quantum confinement effects were then modeled by performing a detailed calculation of the hole subbands in the $Si/Si_{1-x}Ge_x/Si$ quantum wells. In this calculation, we numerically solved the effective-mass equations using an approach suggested by Wessel and Altarelli.[16] Even though we used the full $6 \times 6$ Luttinger–Kohn Hamiltonian[17] including both strain and spin-orbit interactions[18] instead of the reduced $3 \times 3$ Hamiltonian of Wessel and Altarelli,[16] we were able to reduce the problem to finding the roots of a determinant of a $6 \times 6$ matrix rather than $12 \times 12$ as in Ref. 16. Details will be published elsewhere. To carry out the calculation, values of needed parameters were interpolated from those of pure Si and Ge since no experimental data are available for $Si_{1-x}Ge_x$ alloys. For the uniaxial splitting parameter $D_u$, spin-orbit splitting $\Delta$, Poisson ratio $\sigma$, and unit cell volume $a_0^3$, we assume a linear variation between silicon and germanium following People.[19] For the Luttinger valence band parameters $\gamma_1$, $\gamma_2$, and $\gamma_3$, we follow Braunstein,[20] and assume a linear variation of $1/F$, $1/G$, $1/H$, and $1/H_2$, where $F$, $G$, $H_1$, and $H_2$ are k·p parameters originally introduced by Dresselhaus, Kip, and Kittel.[21] That excellent agreement was achieved between the observed shifts in PL band gap and the calculated well width dependency of confinement energy (Fig. 3), justifies our neglect of the confinement effects in the conduction band. The only adjustable parameter was the absolute value of the bulk band gap. A confinement energy of 45 meV is found in the narrowest (33 Å) sample.

For simple engineering calculations the confinement energy was also calculated using a one band effective mass model, with the effective mass in the growth direction (z) of silicon fixed at its heavy-hole value (0.278),[22] and the z-effective mass of the $Si_{0.8}Ge_{0.2}$ given by the result of the above *bulk* calculations (0.264). The results were identical to those predicted by the more complicated approach described above. That the simple theory is applicable is ac-

tually expected in this case: under the strain condition encountered in our samples, for zero in-plane $k_\parallel$ vector, the $Si_{1-x}Ge_x$ heavy-hole band is decoupled from the light-hole and split-off bands,[18] and its bulk dispersion relation $E(k_\parallel = 0, k_z)$ is purely parabolic along the $k_z$ axis. Therefore the Wessel and Altarelli approach reduces to the simple one band model for the heavy-hole ground state, which is what is measured by PL. When $k_\parallel \neq 0$, however, the heavy-hole band is coupled with other bands (as is always the case for the higher-lying light-hole band), and the exact calculation is required to calculate the subband dispersion. The good agreement between our calculations and experiment gives us confidence to predict the heavy-hole effective mass in the z direction of the strained alloys to be used along with $m_z^*$ in the silicon in energy level calculations. This result can be expressed as

$$m_z^* = 0.278 - 0.07x \qquad (1)$$

where $x$ is the Ge fraction.

In summary we have reported the first observation of the quantum confinement shift of band-edge photoluminescence in Si/strained $Si_{1-x}Ge_x$/Si quantum wells. Good agreement is found between the experiment and a theoretical quantum well subband calculation using the $6 \times 6$ Luttinger–Kohn effective-mass Hamiltonian which includes both strain and spin-orbit interactions. Finally, an expression of z-direction heavy-hole effective mass for calculating quantum well energies in the alloys was given.

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