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Intersubband Absorption in Modulation Doped p-type $Si/Si_{1-x}Ge_x$ Quantum Wells: a Systematic Study

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A study of intersubband absorption in modulation-doped p-type Si/SiGe quantum wells is presented for a variety of SiGe-well widths and Ge-contents. Narrow absorption lines (20 meV) between 540 cm^{-1} and 1035 cm^{-1} are observed. If the well width is 30Å, the first excited heavy-hole subband is located close to the top of the quantum well, and we show that a strong mixing occurs between well- and barrier bound states. The latter arise from the hole transfer from the barrier into the well. A self-consistent calculation is used to fit the measured absorption spectra.

The absorption of infrared radiation through intersubband transitions in quantum wells has been studied extensively in the past few years, because of its possible application for infrared detectors[1]. Besides the GaAs/AlGaAs system, the Si/SiGe system has attracted a lot of attention recently. From the technological point of view, it is preferable to employ valence-band transitions in SiGe quantum wells, since the latter can be grown directly on a silicon substrate in a pseudomorphically strained fashion. Even though a number of results on this system have been reported already,[2,3] there is no detailed knowledge yet about the optimum sample parameters (e.g., layer thicknesses, Ge-content) for infrared detection. In this paper we present a study of the hole-intersubband absorptions in SiGe quantum wells for a variety of well thicknesses and depths, the latter being determined by the Ge-content of the alloy material.

The samples investigated in this work were grown by molecular beam epitaxy on semi insulating [100] Si wafers. The samples consist of 10 SiGe alloy quantum wells with a Ge-content of about 30%, separated by 180 Å Si barriers, the center 60Å of which are boron doped to a level of 2.2×10^{18} cm^{-3}. Three groups of samples with different well widths (approximately 30 Å, 50 Å, 70 Å) were grown. During growth, the wafer was not rotated but rather kept fixed. This results in a controlled variation of the Ge-content and well- and barrier-width within one wafer. The exact structural parameters were determined by high-resolution triple axis x-ray diffraction and are listed in Tab.1. The x-ray data show that the SiGe quantum wells are pseudomorphically strained with the in-plane lattice constant of the Si substrate. Infrared absorption

Tab 1: Sample parameters determined by high resolution triple axis x-ray diffraction and FIR transmission measurement. For the 30Å quantum wells, the values in the parentheses were used to obtain the best fit.

Ge cont.	well (Å)	barrier (Å)	Peakpos.(cm^{-1}) meas.	calc.
24	68	179	540	405
20	52	193	690	520
23	51	176	780	610
28	47	162	900	750
19 (20)	36 (35)	180	725	720
25 (24)	30 (30)	177	865	880
29 (29)	26 (30)	160	1035	1060

measurements were performed in a Bruker IFS 113 Fourier transform spectrometer at a temperature of 5 K.The samples were prepared in multipass waveguide geometry (8 reflections at the superlattice) with the facets wedged at an angle of 38° (Ref. 4). On top of the multiquantum well structure a layer of gold (300 nm) was deposited in order to enhance the electric field of the infrared radiation polarized parallel to the growth direction[5]. The transmission spectra were measured both in p- and in s-polarization (electric field parallel / perpendicular to the growth direction). The ratio of the transmitted intensity of p- and s-polarized radiation was normalized to the respective ratio measured at a reference Si substrate prepared in the same way as the multiquantum well samples.

Figure 1 shows the absorption spectra of the 70Å quantum well and the three 50Å quantum wells. The linewidth is about 20 meV, which is only twice

as large as in comparable GaAs quantum wells. The peak positions of the 50Å wells shift from 690 cm^{-1} to 900 cm^{-1} with increasing Ge content (20% to 28%) and decreasing well width (52 Å to 47 Å).In Fig. 2b the transmission spectra of the 30 Å multiquantum wells are shown. Here, the absorption maxima shift from 725 cm^{-1} to 1035 cm^{-1} with increasing Ge-content (19% to 29%) and decreasing well width (36 Å to 26 Å). Furthermore the absorption linewidth is significantly larger than for the other samples. To understand the shape of the absorption lines one has to calculate the energy levels of the multiquantum wells taking into account the electrostatic potential arising from the charge transfer from the doped region of the barrier to the quantum

wells. If we restrict ourselves to the case of zero in-plane wavevector, the energy levels for the heavy holes are the eigenvalues of a one-band Schrödinger equation[6] solved self-consistently together with Poisson´s equation. In the calculation, the band offset of the heavy-hole band in Si and SiGe was treated as a fitting parameter.

As an example, the results of the calculation for a quantum well with a germanium content of 24% and a well width of 30 Å are shown in Fig. 3. Due to band bending, bound states exisit in the barrier. The transitions from the well-bound ground state (labeled 1 in Fig. 3b) to these states (labeled 2, 3 in Fig. 3b) are indirect in real space and therefore have small oscillator strengths. The levels labeled 4 and 5 in Fig. 3b are mixtures between well- and barrier-bound
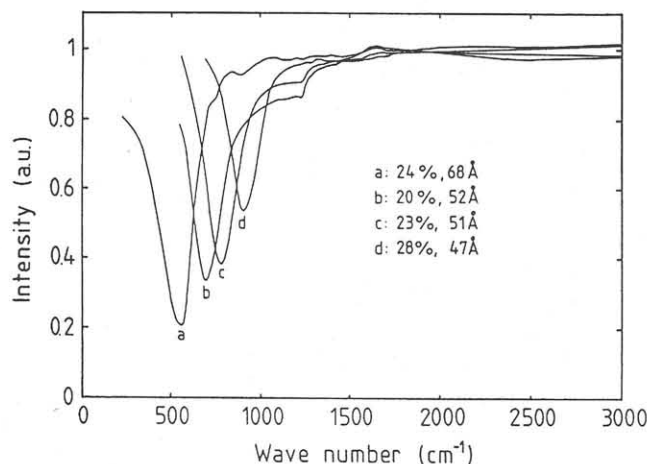

Fig.1: Transmission spectra of four modulation doped p-type Si/SiGe multi- quantum wells measured at 5 K. The respective well width and Ge content is indicated in the plot.
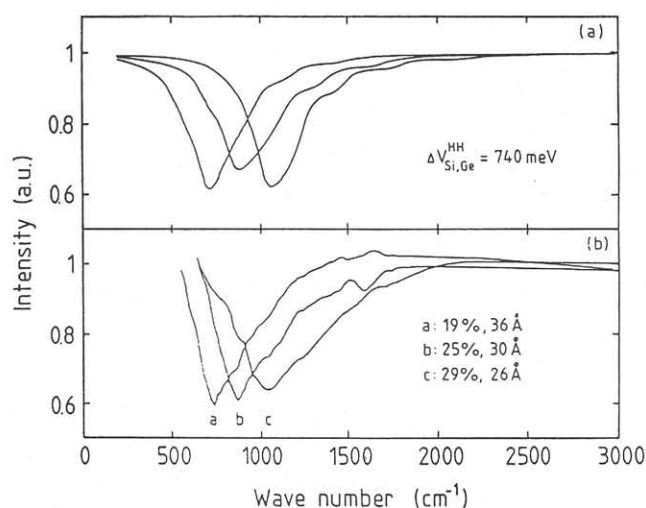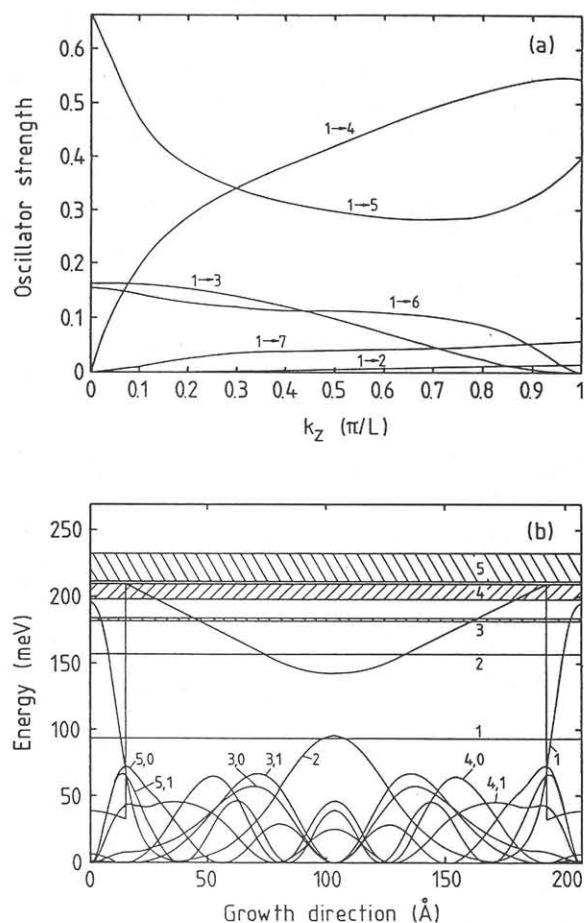

Fig.2: Calculated (a) and at 5K measured (b) transmission spectra of three modulation doped p-type Si/SiGe multiquantum wells. The respective well width and Ge content is indicated in the plot. For the calculation a band offset of 740 meV between the heavy-hole bands of Si and pseudomorphically strained Ge was assumed.

Fig.3: Results of the calculation for a modulation doped multiquantum system with 30 Å $Si_{0.76}Ge_{0.24}$ quantum wells and 177 Å Si barriers. In (a) the oscillator strength for transitions from the ground state to the first 6 excited sates is plotted versus the reduced wavevector along the growth direction (L denotes the period in growth direction). The self-consistent potential and the energy bands are plotted in (b). For convenience, the energy of the holes is counted positive. Also shown in (b) are the wavefunctions of the miniband edge states. The first digit of the labels of the wavefunctions indicate the bandindex, the second the value of the reduced wave vector (in units of π/L).

states. The transitions from the ground state to these states have the highest oscillator strengths (see Fig. 3a) and therefore dominate the absorption spectra. The final states of these transitions are delocalized with a strong dispersion in k_z direction, which results in a rather broad absorption. The transitions in the 30Å quantum wells are most sensitive to the valence band offset, since the excited states with the highest oscillator strength have energies close to the top of the quantum well. Consequently, the absorption spectra of these samples were used to determine the valence band offset. Using a heavy-hole valence band offset of 740 meV between Si and pseudomorphically strained Ge (and linear interpolated values for the alloy (Ref.7)), we calculated the transmission spectra plotted in Fig. 2a. The results of the calculation not only reproduce the positions of the measured absorption maxima, but also the structures observed in the high energy shoulder of the absorption band (especially for the quantum well with 25% Ge content). We point out that it is crucial to take into account transitions to several excited states, which all contain considerable oscillator strength. For the 50 Å and 70 Å samples, however, the results of the calculation do not coincide well with the experimental results (see Tab.1). The reason for this discrepancy is not clear yet, but could be caused by intersubband transitions with finite in-plane wavevector values which are not taken into account in the present calculation.

To summarize, we have performed a systematic experimental study of the infrared absorption of modulation doped p-type Si/SiGe quantum wells with various Ge-content and well widths. As long as the wavefunctions of the excited states do not couple to continuum states, the linewidth of the aborption is only 20 meV, showing the high quality of the present samples. For the 30 Å samples, the results of a model calculation agree very well with the experimental results, if a band offset of 740 meV between Si and pseudomorphically straind Ge is assumed.

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