Optical Characterization of Self-Assembled Si/SiGe Nano-Structures

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Self-assembled SiGe nano-structures buried under a Si cap layer have been investigated by infra-red absorption and photoluminescence spectroscopy. Together with results of x-ray diffraction and reflection experiments, from these experiments detailed information about the alloy concentration in and the size of the nano-structures is obtained.

1. Introduction

The optical properties of low dimensional structures in the Si/SiGe system are of special interest since by integrating such structures in standard Si technology it is possible to add optoelectronic performance to mainstream material for integrated circuits. The self-organized growth of nano-structures (i.e. Stransky-Krastanow growth mode for quantum dots, step bunching along the terraces of a vicinal substrate for quantum wires) appears to be very appealing, since by these methods rather uniform nano-structures with high density can be achieved without structuring the samples for example by photo- or electron-lithography. However, since the self-assembling is a statistical process, the size and the alloy concentration of the nanostructures are statistically distributed. Therefore, a sensitive characterization of the structural parameters of the nano-structures is essential. For possible future applications, the nanostructures have to be overgrown, and surface scanning methods are not applicable for the characterization of these structures. We show that in addition to x-ray diffraction, absorption, and photoluminescence experiments are valuable tools for the non-destructive characterization of overgrown nano-structures.

2. Experimental

In this work we have performed infrared transmission (TR) experiments for the structural characterization of SiGe quantum dots (QD) formed by the Stranski-Krastanow mode on a SiGe wetting layer and photoluminescence (PL) experiments for the characterization of SiGe quantum wires (QWR) grown by step bunching along terraces of a vicinal Si substrate.

The SiGe QDs were grown by solid-source molecular beam epitaxy on an insulating Si substrate at a substrate temperature of T = 525 °C and a Ge deposition of 8 monolayers. The samples consist of 30 QD layers separated by 50 nm Si barriers. The nominal dot

height (3 nm), diameter (35 nm) and density (6 x 10^{10} cm^{-2}) were determined by atomic force microscopy on reference samples without a Si cap. The samples are p-type (Boron) modulation doped to a level of approximately 4 holes per dot.

Transmission experiments were performed in waveguide geometry with the sample facets wedged at 30° (see inset of Fig. 1) and gold evaporated on the sample surface. In Fig. 1, the ratio of TR measured in TM and TE polarization is shown. The spectra were measured at the temperatures indicated in the plot and normalized to the respective ratio of spectra measured at room temperature in order to remove a wavelength dependent background. For clarity, the curves are vertically shifted by -0.005 for each measurement at lower temperature. An absorption line centered around 260 meV is clearly observed. Model calculations described in Ref. [1] show that the absorption is due to hole transitions between the heavy hole (HH) ground state and the first excited HH state resulting from the confinement in growth direction.

In lateral photocurrent (PC) experiments performed on the same samples, transitions to delocalized continuum states are observed, resulting in an onset of the photo signal at a higher energy than the onset of the absorption observed in the TR experiment (transitions to bound states) [1]. By comparing the measured transition energies to both the confined and continuum states to the model calculations described in [1] it is possible to estimate both the average Ge content (65% – 75%) and the dot height (27 Å). These results show that even at the moderate growth temperatures used for the samples investigated in this work, significant alloying occurs during the overgrowth of the dot layers.

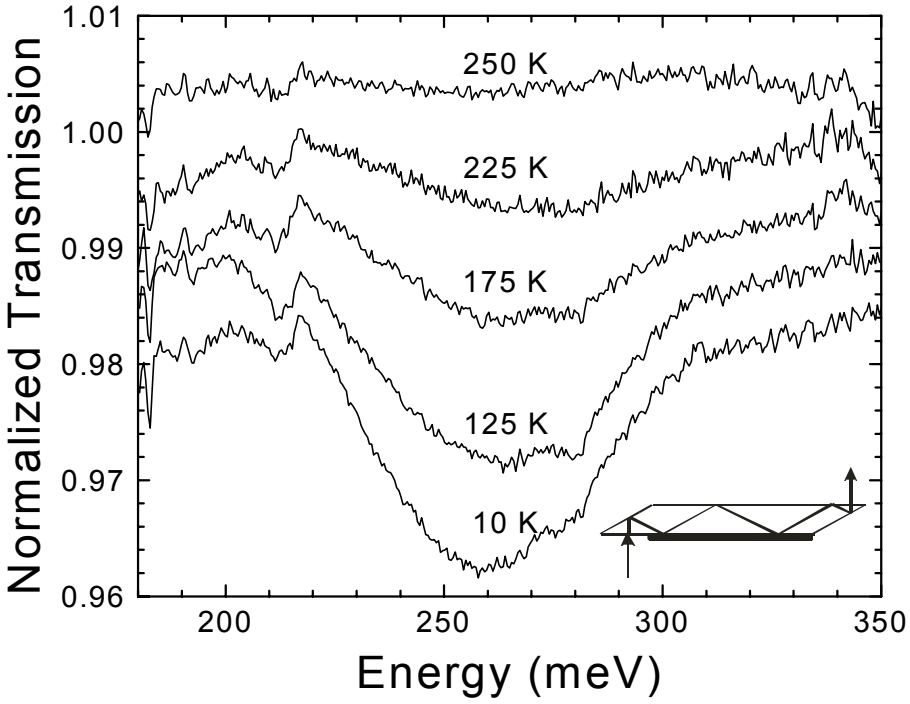

Fig. 1: TR spectra of the SiGe QD sample measured in waveguide geometry at the temperatures indicated in the plot. On the ordinate axis, the ratio of TR measured in TM and TE polarization normalized to the respective ratio measured at room temperature is plotted. For clarity, the spectra are vertically displaced by -0.005 for each temperature step.

The structural properties of a series of SiGe quantum wires (QWR) grown on vicinal (001) Si substrates have been investigated by x-ray diffraction and PL measurements [2]. The samples consist of 20 periods of nominally 25 Å thick $Si_{1-x}Ge_x$ layers separated by 100 Å Si layers. The nominal Ge content of the alloy layers is 0.35, 0.40, 0.45 for samples A, B and C, respectively. In order to initiate step bunching, and the wire growth, a vicinal (001) Si substrate with a rather large miscut angle of 3.5° towards [100] direction was chosen. All samples were capped with a 100 Å Si layer. The details on the MBE growth are given in Ref. [3]. The results of the x-ray experiments [2] clearly indicate that the wires have a triangular cross section with a base length of about 350 Å and a facet angle of 6°. The wires have assembled on top of a SiGe wetting layer (WL) with a thickness of approximately 25 Å and a Ge concentration 0.33.

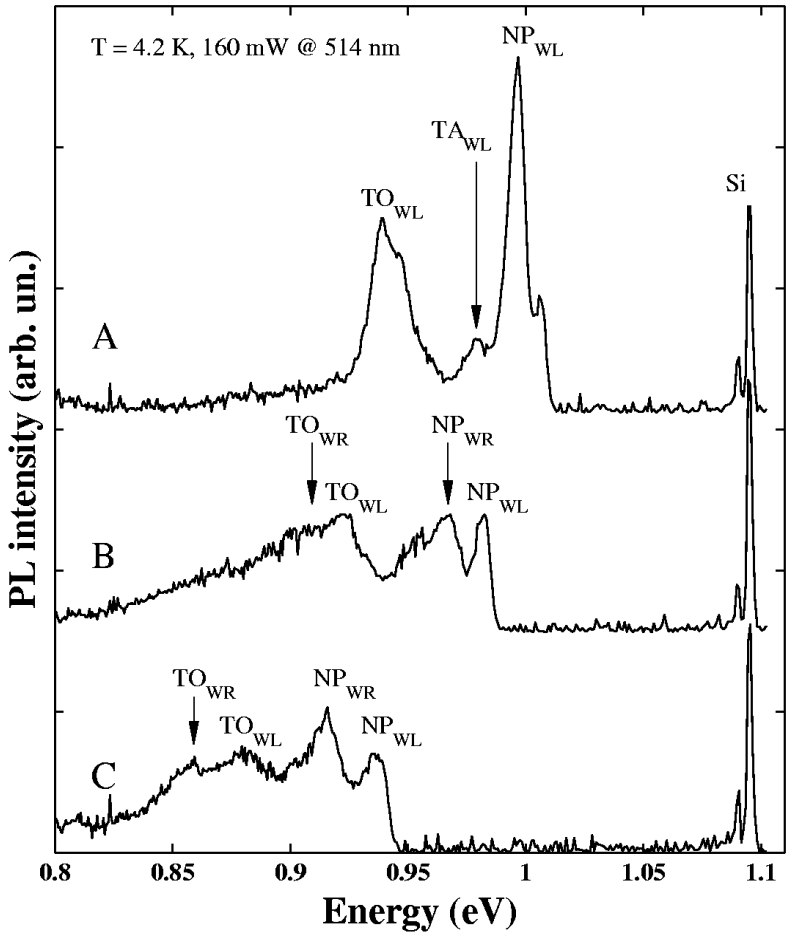

Fig. 2: Photoluminescence spectra of samples A,B, and C. The PL peaks are labeled according to the type of phonons involved in the exciton recombination (NP: no phonon, TO: transverse optic, TA: transverse acoustic) with a subscript indicating where the recombination occurs. (WL: wetting layer, WR: quantum wire).

Low temperature (T = 4.2 K) PL spectra of samples A,B, and C are shown in Fig. 2. The PL was excited by the 514 nm line of an Ar^+ laser with an intensity of 0.8 W/cm^2. The spectrum of the sample with the lowest Ge content (A) is typical for a 2 dimensional

SiGe quantum well layer. The lines at 0.997 eV, 0.979 eV and 0.940 eV (labeled NP_{WL} TA_{WL} and TO_{WL} in Fig. 2) are commonly attributed to the no-photon luminescence of a SiGe quantum well exciton and its transverse-acoustic and transverse-optical phonon replica. No indication of PL from quantum wires is observed in the spectrum of sample A. Therefore, we conclude that in this sample no quantum wires have formed and the observed PL is due to recombination of excitons confined to the WL only. Also in the x-ray experiments, no diffraction pattern characteristic for QWR is observed for this sample. The PL spectra of the samples with the higher Ge content (B, C) significantly differ from the spectrum of sample A: In addition to the strongly quenched NP_{WL} line and its phonon replica, new PL peaks appear in the spectra: a broad PL line (labeled NP_{WR}) is observed approx. 20 meV below the NP_{WL} line. This peak dominates any contribution of the TA_{WL} line possibly present in the spectra of samples B and C. We assign the NP_{WR} peak to PL from excitons confined to the self-organized quantum wires. For the sample with the highest Ge content investigated in this work (C), the NP_{WR} becomes the strongest signal in the PL spectrum. In addition to the NP_{WR} peak, a line labeled TO_{WR} is clearly resolved in the spectrum of sample C. Since this line is shifted to lower energies by the energy of a Si-Si TO phonon (58 meV) with respect to the NP_{WR} peak position, we assign it to a TO phonon replica of the NP_{WR} line. For sample B, the TO_{WR} signal is less pronounced and appears as a shoulder in the PL spectrum. Using the energy difference between the NP_{WL} and NP_{WR} lines observed in the luminescence spectra of sample B and C (20 meV), we have estimated the Ge concentration in the SiGe QWRs by calculating the confinement energies in the WL and in the QWR. Since the extension of the wires in lateral direction is approx. 10 times larger than in vertical direction, in the calculations we neglect the lateral confinement and model the quantum wire structure consisting of the WL and the self-assembled wire part by a two dimensional step quantum well. In Ref. [2] it is shown that within this model the small energy difference of 20 meV can be explained if Ge concentration in the range between 20% – 30% is assumed in the QWR, i.e. a *smaller* Ge concentration than determined for the WL by x-ray diffraction (33%). This unexpected finding is in excellent agreement with the results of x-ray measurements, which indicate 20 ± 10% Ge concentration in the QWR [2].

3. Conclusion

By carefully analyzing TR, PC and PL spectra we have shown that significant alloying occurs during the overgrowth of self-assembled SiGe quantum dots even at moderate growth temperatures around 525 °C. In addition we have shown that unlike in SiGe QDs, where the Ge content is usually higher in the self-assembled dots than in the WL, in the QWRs investigated in this work the WL contains a higher Ge fraction than the self-assembled wires.

Acknowledgements

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References

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