Identifying spins states on self assembled Si/SiGe quantum dots by means of ESR

F. Lipps, F. Pezzoli, M. Stoffel, Ch. Deneke, J. Thomas, A. Rastelli, V. Kataev, O. G. Schmidt, B. Büchner
Institute for Solid State and Materials Research, IFW Dresden, P. O. Box 270116, D-01171 Dresden, Germany
E-mail: f.lipps@ifw-dresden.de

Abstract. Self-assembled Si/SiGe quantum dots were systematically studied with ESR at 9.56 GHz. A set of multilayer structures were grown with molecular beam epitaxy with different vertical spacing between quantum dot layers and different dot sizes. An extensive characterization with transmission electron microscopy and atomic force microscopy provides good structural information of the ensembles of quantum dots. Furthermore the samples were characterized by photoluminescence. Two ESR signals were identified with $g$-factors around 1.9992 and 1.9994. Both signals show a small anisotropy in $g$-factors and linewidth with respect to the magnetic field along growth and in-plane directions. Spin-relaxation times $T_1$ are determined with continuous wave ESR saturation measurements to be of the order of 10 µs. The spin dephasing times yield values up to 500 ns. Illumination with sub-bandgap light changes the relative intensity of the two signals. Based on calculations of the electronic structure of the heterostructures a qualitative model allows us to relate the two ESR signals to s- and p-like-states on the quantum dots.

1. Introduction
The spin-orbit coupling in IV-IV semiconductors is fairly weak. Therefore long spin lifetimes and coherence times are expected, opening opportunities for spintronic applications in Si-based systems. Because of the indirect bandgap of Si and Ge, the use of optical methods, which have proved powerful to study spin states in the case of III-V materials, is limited. Electron spin resonance (ESR) is a technique, which allows to determine static and dynamics of spin ensembles also for Si-based heterostructures [1]. Specifically, continuous wave ESR can provide information about the $g$ factor as well as relaxation and dephasing times of a spin system.

2. Results
Two sets of samples were grown by means of molecular beam epitaxy (MBE) at temperatures of 600 °C and 700 °C respectively. The samples consist of fourfold-stack of SiGe quantum dots embedded in a Si matrix. The spacing between the quantum dots is varied from 20 to 100 nm. More details are given elsewhere [2].

ESR experiments were performed with a Bruker EMX spectrometer around a frequency of 9.56 GHz in a resonator with optical access at temperatures around 4 K. Because of the small spin-orbit coupling in Si-based systems the $g$ factor of electrons is expected...
Figure 1. (a) ESR spectra for samples grown at 600 °C and (b) 700 °C with the magnetic field in (001) growth direction and perpendicular to it. Only a broad single peak is observed for 600 °C, while there are two peaks for 700 °C-sample. (c) linewidth and (d) g factor as a function of magnetic field direction. The g factor can only be determined in the range where the lines are resolved to be close to the g factor of the free electron $g \approx 2$. ESR signals could be identified in all quantum dot samples with a g factor of about 1.999. Careful measurements of reference samples without quantum dots confirmed that these signals are indeed associated with the quantum dots (for details see [2]). In this paper we will focus on samples with 70 nm vertical spacing. While there is only a single peak visible for the samples grown at 600 °C around a g factor $g_0 = 1.9992$ [Fig.1(a)] two peaks are identified in the structures grown at 700 °C with g factors $g_{0,R} = 1.9992$ and $g_{0,L} = 1.9994$ - for a magnetic field applied in the (001) growth direction [Fig.1(b)]. From the linewidth the dephasing time $T^*_2$ can be calculated [3] and amounts, for the 700 °C sample, to up to 500 ns. By measuring the ESR-intensity as a function of applied microwave power the relaxation time $T_1$ can also be calculated [3]. $T_1$ is estimated to be slightly shorter than 10 $\mu$s in all structures investigated.

As the external magnetic field is turned in-plane the lines broaden [Fig.1(c)] and in case of the former two peak spectra the peaks cannot be distinguished anymore [Fig.1(a),(b)]. However the different relative intensities make a characterization of the linewidth possible. Also the g factors show an anisotropic dependence regarding growth direction and quantum dot plane. However, this anisotropy is fairly small [Fig.1(d)] and is within the error of the measurements. The same holds for peak R in both structures.

The Si/SiGe quantum dots were modelled with the program NEXTNANO$^3$ [4]. Structural information extracted from transmission electron microscopy (TEM) and atomic force microscopy (AFM) were used to implement shape and intermixing profile of the quantum dots in the simulations. Elastic strain and single band effective mass calculations were carried out. In agreement with previous publications [5, 6] the band structure shows a type II band alignment. As a consequence electrons are confined at the apex of the dot in the lowest lying conduction band of
the Si matrix, the $\Delta_2$ band, while holes are confined inside the SiGe dot. The occupation of the quantum dots depends on the number of donors per dot. In addition it also depends on the ionization energies of those dopants, which determine the Fermi energy at a given temperature, with respect to the quantum dot eigenstates. The intrinsic ($n$ type) background doping gives an average occupation on the order of 10 donors per dot. However, since the donor ionization energy (45 meV for phosphorus) is close to the lowest quantum dot eigenstate not all electrons are trapped on the dots.

For the two sample sets the Ge concentration in the dots and their size are different and

![Figure 2.](image)

**Figure 2.** (a) strain profile of a modelled semi-parabolic quantum dot. The z-axis is along the (001) growth direction. (b) eigenvalues for different quantum dots, 80, 120 and 200 nm refer to their basediameters

![Figure 3.](image)

**Figure 3.** (a) probability wavefunctions of the s-state for 80 nm [(i), (ii)] and 120 nm dot basdiameter [(iii), (iv)]; probability wavefunction of p-state for magnetic field in xy-plane [(i), (ii)] and z-direction [(iii), (iv)] direction for dot basediameter of 120 nm

with that eigenstates and eigenfunctions differ. Samples grown at 600 °C show a base diameter of about 80 nm while samples grown at 700 °C are significantly larger having base diameters
of about 200 nm. Because of that the energy spacing between s- and p-states is significantly decreased from $>2 \text{meV}$ for the small dots to about 0.4 meV for the large ones (Fig. 2(b)). The structures consist of a large ensemble of dots where the individual energy levels vary slightly throughout the sample. At temperatures around 4 K, as used in the experiments, a thermal population of p-states, in addition to population of s-states, is therefore possible in the bigger dots. With an increase in size of the confining potential also the size of the electron wavefunction is increasing. However, the pancakelike shape (s-state) is preserved. This is nicely visible in Fig. 3(a), which shows the s-state probability wavefunctions of quantum dots with 80 nm [(i),(iii)] and 120 nm base diameter [(ii),(iv)]. While there is no influence of a magnetic field on the s-states the p-state is distorted when the magnetic field is turned from the plane [Fig. 3(b)(i),(ii)] to the growth direction [Fig. 3(b)(iii),(iv)].

The illumination with light below the bandgap of Si increases only the right peak $R$ (not shown - see Ref. [2]). This can be understood as an ionization of donors or a direct generation of carriers from the quantum dot. With that an increase in the quantum dot occupation is reached. Therefore, the right peak $R$ is identified as the quantum dot p-state.

3. Summary & Conclusion
A systematic ESR study on Si/SiGe heterostructures was performed. The ESR signals could be identified as s- and p-like-states at the quantum dots. $g$ factor and relaxation times were characterized. The timescales for $T_1 \approx 10 \mu s$ and $T_2 > 500 \text{ns}$ are shorter than those of electrons on donors in Si [7], but sufficiently long to allow spin manipulation with established ESR techniques.

Acknowledgements
Support by DFG through FG-912 is gratefully acknowledged.

References
[1] Malissa H, Jantsch W, Chen G, Gruber D, Lichtenberger H, Schäffler F, Wilamowski Z, Tyryshkin A M and Lyon S 2006 Materials Science and Engineering: B 126 172–175
[2] Lipps F, Pezzoli F, Stoffel M, Deneke C, Thomas J, Rastelli A, Kataev V, Schmidt O G and Bächner B 2010 Phys. Rev. B 81 125312
[3] Poole Jr C P 1996 Electron Spin Resonance: A Comprehensive Treatise on Experimental Techniques 2nd ed (Dover Publications, Inc.)
[4] Birner S, Zibold T, Andlauer T, Kubis T, Sabathil M, Trellakis A and Vogl P 2007 IEEE Trans. Electron Devices 54 2137–2142
[5] Schmidt O G, Eberl K and Rau Y 2000 Phys. Rev. B 62 16715
[6] Grützmacher D, Fromherz T, Dais C, Stangl J, Müller E, Ekinci Y, Solak H H, Sigg H, Lechner R T, Wintersberger E, Birner S, Holy V and Bauer G 2007 Nano Letters 7 3150–3156
[7] Feher G and Gere E A 1959 Phys. Rev. 114 1245