Summary

The simultaneous detection of two dangling bond centres at and below a (100) Si/SiO_2 interface is reported for the first time. It is noted that the detected dangling bond centre P_{ba} is very similar to the P_{b0} defect reported in the literature. The P_{b0} centre is related to implantation damage below the Si/SiO_2 interface, leading to dangling bonds within the bulk material. Assuming a positive identification of P_{ba} with P_{b0} the result underlines the observation that the P_{b0} centre is generated by particle radiation. However, the identification of the P_{ba} centre found here with the known P_{b0} centre must remain somewhat uncertain.

The more anisotropic P_{bb} centre can be attributed to dangling bonds at the (100) Si/SiO_2 interface, occurring after annealing or low energy particle implantation. The Electrical Detection of Electron-Paramagnetic Resonance (EDEPR) signal of the P_{bb} centre can be increased by annealing in an oxygen containing atmosphere. The P_{bb} centre has been detected for the first time due to the increased sensitivity and low noise figure of low temperature EDEPR measurements.

Angular dependent EDEPR spectra of the dangling bond centres P_{ba} and P_{bb} have been recorded with improved spectral resolution and signal-to-noise ratio. The calculation of the angular dependence reveals a threefold symmetry of both defects. It can be concluded that the dangling bonds are aligned along a [111] direction in the crystal. The P_{ba} centres are thought to be due to silicon vacancies in the bulk created by radiation damage leaving the [111] dangling bond at one neighbour. The radiation damage is also believed to stabilise the vacancies against diffusion.

Shallow thermal donors which were prepared according to a recently developed procedure, comprising hydrogenation and electron-irradiation prior to annealing, were investigated with optical and magnetic resonance spectroscopy. Thus, three species (D1-D3) of these shallow donors can be created selectively by choosing a specific temperature in the range of (300–500)°C for the annealing step. The electronic properties of the D*n*

were determined by means of Fourier Transform Infrared Absorption (FTIR) measurements. Evidence for an identification of D2 and D3 with two species of hydrogen-related shallow thermal donors (STD(H)) reported in the literature was found from the FTIR data. It is shown that the D1 is a precursor or the first species of the STD(H), undiscovered before.

EPR studies of the D*n* centres revealed an isotropic (g = 1.9987) D1 signal upon rotation of the sample and orthorhombic-I symmetry for D2 centres ($g_{x,y,z}$ = 1.99952, 1.99722, 1.99982, Δg = ±0.00002). The high accuracy of the g-values was obtained from EDEPR spectra recorded with V-band microwaves (72GHz). The g-values of the D2 are very similar to those of the oxygen precipitate NL10 presented in the literature and an identification of the D*n* with the early species of the NL10 is suggested. Hyperfine (hf) lines of D1 and D2 due to an interaction of the unpaired electron with ^{29}Si nuclei (nuclear spin I=1/2) are observed. From the intensity ratio of the hf lines to the central line (≈ 5%) the incorporation of one silicon atom in the defect structure of the D*n* is concluded. Similar hf interactions are observed for NL10 defects with the incorporation of hydrogen, NL10(H), and aluminium, NL10(Al) for the first time.

The detection of the individual D*n* centres with both methods FTIR and EPR provides a clear link between the STD(H) and the NL10(H) centres, reported in the literature separately from measurements of FTIR and EPR, respectively.

From an Electron-Nuclear Double Resonance (ENDOR) study of D1 centres prepared with hydrogen (deuterium), the incorporation of one hydrogen (deuterium) atom in the D1 defect is found. The angular dependence of the ENDOR spectra can be understood assuming a low symmetric (triclinic) hf tensor of the hydrogen atom. From the hf interactions observed in ENDOR a very low spin density at the site of the hydrogen is derived. A comparison with published data reveals that with the investigation of the D1 centre the first species of the STD(H) / NL10(H) has been studied for the first time.

An atomic model for the STD(H) centre had been presented previously on the basis of theoretical calculations. All experimental findings of this study support the suggested $(C\text{-}H)_i\text{-}Si_s\text{-}O_{2i}$ structure. Furthermore, as an interstitial site for the Al-atom in NL10(Al) was suggested in a previous study, a similar atomic model with the $(C\text{-}H)_i$ exchanged by an Al_i can be proposed for the NL10(Al).

Finally, the results of the EDEPR measurements carried out for this thesis have been summarised. A previously suggested donor-acceptor pair (DAP) recombination model for the mechanism of EDEPR was used to explain the recorded spectra. An investiga-

tion of the characteristic microwave power dependence of the EDEPR signals and both the sign and the magnitude of the conductivity change support the assumption. Further, indications were searched for to explain an amplification of EDEPR signals after irradiation of silicon samples with electrons. It is concluded that by the creation of the radiation-induced defect SL1, which appears upon illumination of the sample, an efficient recombination channel is provided via the triplet state of the SL1. This recombination channel can be “used” similar to a “shunt” known from Optically Detected Magnetic Resonance by other defects in the sample and their EDEPR signal can be significantly increased.

Further it is shown that a variation of the modulation techniques for the detection of EDEPR can improve both the signal-to-noise ratio of the detected signals and the spectral resolution in the case of several overlapping resonance lines. The spectral resolution of EDEPR was further enhanced by the use of high microwave frequencies in a modified high-field spectrometer. EDEPR measurements with frequencies as high as 72GHz are reported for the first time.