Giant Anisotropy of Zeeman Splitting of Quantum Confined Acceptors in Si/Ge

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Shallow acceptor levels in Si/Ge/Si quantum well heterostructures are characterized by resonant-tunneling spectroscopy in the presence of high magnetic fields. In a perpendicular magnetic field we observe a linear Zeeman splitting of the acceptor levels. In an in-plane field, on the other hand, the Zeeman splitting is strongly suppressed. This anisotropic Zeeman splitting is shown to be a consequence of the huge light-hole–heavy-hole splitting caused by a large biaxial strain and a strong quantum confinement in the Ge quantum well.

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Spintronic and quantum computing [1,2] are novel device concepts relying on quantum mechanical coherence. Si/Ge-based systems are promising candidates offering long spin coherence times [3,4], fast operations, and a well-established record of scalable integration. These important properties are also crucial requirements [2,5,6] for implementing multiqubit operations in a future quantum computer. One concept that may form the technological basis of a quantum computer is the spin-resonance transistor (SRT) [7]. Vrijen *et al.* [8] proposed a SRT where the electron spin manipulation is realized using the change in g factor between Si-rich and Ge-rich environments of a Si/Ge heterostructure. However, engineering the g factor [9,10] in such systems is complicated by the fact that the electron states in Si are in the X valleys whereas in Ge the electrons are located in the L valleys [11]. This problem does not arise for the valence band states, as both Si and Ge have their valence band maximum at the Γ point. Thus, valence band states in Si/Ge are a promising choice [12] for g-factor engineering in the search for spin manipulation.

In this Letter we have analyzed the g factor of shallow acceptor levels in a Si/Ge heterostructure by resonant-tunneling spectroscopy. We find that their effective g factor is highly anisotropic, giving a large Zeeman splitting of the acceptor states in a perpendicular field, whereas we cannot resolve any Zeeman splitting in in-plane fields up to 18 T. This giant anisotropy, which is much larger than in other systems [13–16], provides the possibility to tune the coupling of the holes to an external magnetic field by a gate-controlled shift of the hole wave function [17] in spintronic devices.

For a proper understanding of acceptor levels it is essential to take into account the fourfold degeneracy of the valence band at the Γ point (Fig. 1) which reflects the fact that the bulk valence band edge in these materials is characterized by an effective angular momentum $J = 3/2$ [18,19]. As the symmetry of the crystal is reduced due to biaxial strain and a confinement potential, the degenerate states split into heavy-hole (HH) subbands with $J_z = \pm 3/2$ and light-hole (LH) subbands with $J_z = \pm 1/2$. Here, the quantization axis for the angular momentum is the z axis perpendicular to the epitaxial layer. So both parameters, the confinement potential, and the built-in strain substantially influence the energy levels of an acceptor in a quantum well (QW) [20,21]. In a magnetic field $B_\perp$ orientated perpendicular to the epitaxial layer we get a Zeeman splitting of HH and LH states, $\Delta E^{\perp}_{\mathrm{HH(LH)}} = g^{\perp}_{\mathrm{HH(LH)}} \mu_B B_\perp$, where $g^{\perp}_{\mathrm{HH(LH)}}$ is the g factor of the HH (LH) states in a perpendicular field and μ_B is the Bohr magneton. But for an in-plane magnetic field $B_\parallel$ the linear Zeeman splitting of HH states is suppressed because there is no $B_\parallel$-induced direct coupling between these states, $\langle \mathrm{HH} | \boldsymbol{J} \cdot \boldsymbol{B}_\parallel | \mathrm{HH} \rangle = 0$, where $\boldsymbol{J}$ is the vector of $J = 3/2$ spin matrices [22–25]. This does not apply for LH states, which show a significant Zeeman splitting $\Delta E^{\parallel}_{\mathrm{LH}} > 0$. We emphasize that the vanishing Zeeman splitting of HH states in a parallel field reflects the fact that the HH-LH splitting in our samples is much larger than the maximal Zeeman energies (~7 meV) [19].

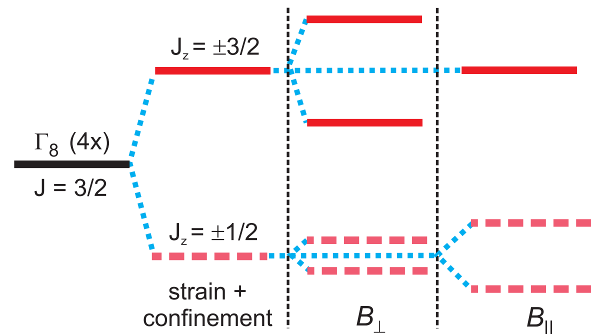

FIG. 1 (color online). Qualitative sketch of the valence band states at different perturbation conditions. Already at $B = 0$, biaxial strain and a confinement potential reduce the fourfold degeneracy to twofold, giving heavy-hole (HH) states with $J_z = \pm 3/2$ and light-hole (LH) states with $J_z = \pm 1/2$. Depending on the orientation of the magnetic field, the twofold degeneracies of the HH and LH states will be lifted or preserved.

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Figure 2 shows the layer sequence and the valence band profile of our samples. They are prepared by growing a 100 nm thick Si:B layer ($p = 8 \times 10^{18}$ cm^{-3}) on a (001) p^+-Si substrate. The active region of the samples consists of two 10 nm thick SiGe QWs separated by a 10 nm thick Si barrier. In the center of the Si barrier a 4 monolayer (ML) thick Ge QW is embedded. Finally, the active region is capped with 100 nm Si:B ($p = 8 \times 10^{18}$ cm^{-3}). For the dc-transport measurements we have fabricated diodes with lateral diameters of 1 μm. Measurements were performed at temperatures down to $T = 50$ mK and using magnetic fields up to 18 T.

Figure 3(a) shows a typical current-voltage (I-V) characteristic of a diode at $T = 50$ mK. A staircase structure is observed that is even better resolved in the differential conductance (dI/dV) curve shown in Fig. 3(b). The step-like increase of the current is in a bias range which is about 300 mV below the onset of resonant tunneling of holes through the 2D subbands of the central Ge QW, so that this mechanism cannot explain the current steps. We attribute these current steps in the pA range to tunneling processes of heavy holes through zero-dimensional acceptor levels of Boron dopant atoms which have migrated into the Ge QW from the highly doped Si:B contact regions.

Similar to resonant tunneling of electrons into zero-dimensional states of quantum dots or shallow donors (see, e.g., Refs. [16,26]), our current steps result from tunneling of heavy holes from the SiGe QW through acceptor levels E_s in the Ge QW (see Fig. 2). A resonant-tunneling process through an acceptor level E_s occurs each time E_s is in resonance with the Fermi energy E_F of the SiGe emitter. The bias position of a current step is given by $V_s = (E_s - E_F)/\alpha e$, where α is the bias-to-energy conversion coefficient. We determine α from the temperature-dependent broadening of the current step edges. As a measure of this broadening, we use the full width at half maximum of the corresponding differential conductance peaks, ΔV_s [see Fig. 3(b)]. It increases according to $(\alpha e \Delta V_s)^2 = (\Delta E_s)^2 + (3.53kT)^2$, where the term $3.53kT$ stems from the broadening of the Fermi function characterizing the carrier distribution. Using this equation we obtain $\alpha = 0.5 \pm 0.1$ for several peaks in both bias polarities.

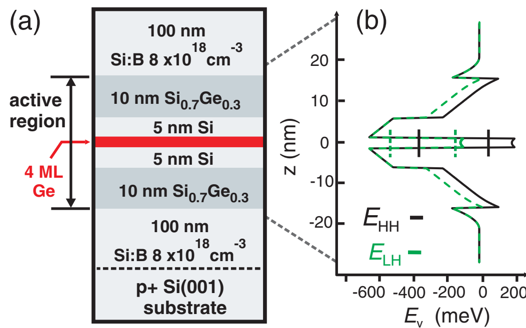

FIG. 2 (color online). (a) Layer sequence of the heterostructure. (b) Self-consistently calculated valence band profile of the active region. The solid line shows the shape of the heavy-hole (HH) subband and the dashed line the light-hole (LH) subband. Because of biaxial strain and a strong quantum confinement a huge HH-LH splitting results.

Figure 4 shows a gray-scale plot of the differential conductance dI/dV as a function of an external magnetic field orientated perpendicular to the epitaxial layer, $B_\perp$. In the voltage range from -15 to 15 mV the conductance maxima exhibit a linear splitting as a function of $B_\perp$. All levels show accurately the same splitting, as indicated by the parallel evolution of the conductance maxima. As an example, the upper panel of Fig. 4 shows the splitting of the conductance maximum at 6.5 mV. The gradient of the splitting is $d\Delta V_Z/dB_\perp = 0.73$ mV/T. We attribute the linear splitting to the Zeeman splitting of the HH sublevels, $\Delta E_Z = g_{HH}^\perp \mu_B B_\perp$. The g factor $g_{HH}^\perp$ can be determined using

$$g_{HH}^\perp = \frac{\alpha e}{\mu_B}\frac{d\Delta V_Z}{dB_\perp}. \tag{1}$$

With $\alpha = 0.5$ and $d\Delta V_Z/dB_\perp = 0.73$ mV/T we obtain $g_{HH}^\perp = 6.3$. This value agrees well with optically measured g factors [27,28] of group-III impurities such as B in Ge. This confirms the assumption that the observed levels belong to Boron dopant atoms which have diffused from the heavily doped contact regions into the Ge QW.

Using the $B_\perp$ dependence of the conductance we can obtain an upper limit for the radial extent λ of the wave function of a hole bound to an acceptor level. According to first-order perturbation theory, a ground state acceptor level is affected by a diamagnetic shift $\Delta E_D \simeq e^2 B_\perp^2 \lambda^2/8m^*$, with $m^* \approx 0.28m_0$ the HH effective mass

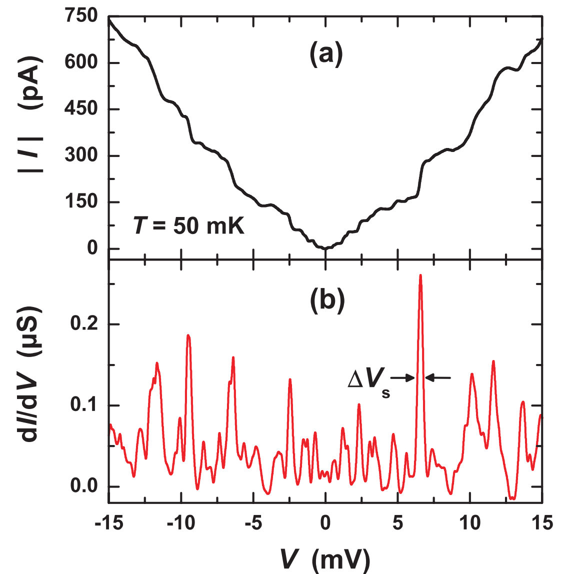

FIG. 3 (color online). (a) Current-voltage (I-V) characteristics of a diode with a diameter of 1 μm at $T = 50$ mK and (b) the corresponding differential conductance (dI/dV). A current step (a) and a differential conductance peak (b) occur whenever resonant tunneling through a shallow acceptor level in the Ge quantum well is energetically possible.

of Ge. (We neglect here the modifications of the hole wave functions caused by the confinement in the narrow QW.) But even at $B_\perp = 18$ T a diamagnetic shift of the levels cannot be observed in our measurements, only the contribution of the linear Zeeman splitting can be seen in Fig. 4. This implies that the diamagnetic shift ΔE_D of the acceptor level is smaller than the width $\Delta E_s \simeq 0.15$ meV of the conductance peak at 50 mK so that λ must be smaller than 2.5 nm. Therefore, λ of the acceptor wave functions in the thin Ge QW is of the same order as the QW width. We remark that Bastard [29] derived a simple model to estimate λ for an impurity in a narrow QW which yields for our system parameters $\lambda \approx 0.8a_B^*$, where $a_B^* \simeq 3.1$ nm is the effective Bohr radius for heavy holes in Ge.

Next we present in Fig. 5 our results for the measured conductance in an *in-plane* magnetic field $B_\parallel$. While we saw in Fig. 4 that $B_\perp$ gives rise to a significant Zeeman splitting of the acceptor levels linear in $B_\perp$, it is most remarkable that up to 18 T most conductance maxima are not at all influenced by an in-plane magnetic field $B_\parallel$. The conductance maximum at 6.5 mV, which exhibits a pronounced linear splitting for $B_\perp$ (arrow in Fig. 4), does not show any splitting in the case of an in-plane magnetic field $B_\parallel$ (arrow in Fig. 5). If a splitting exists, it must be smaller than the width of the conductance peak which is about 0.35 meV [30] here. Another $B_\parallel$-induced effect, which is less easily recognized in Fig. 5, is the suppression of the conductance peaks, as expected for this magnetic field orientation [31]; e.g., at 18 T the peak marked by the arrow is reduced by around 20%.

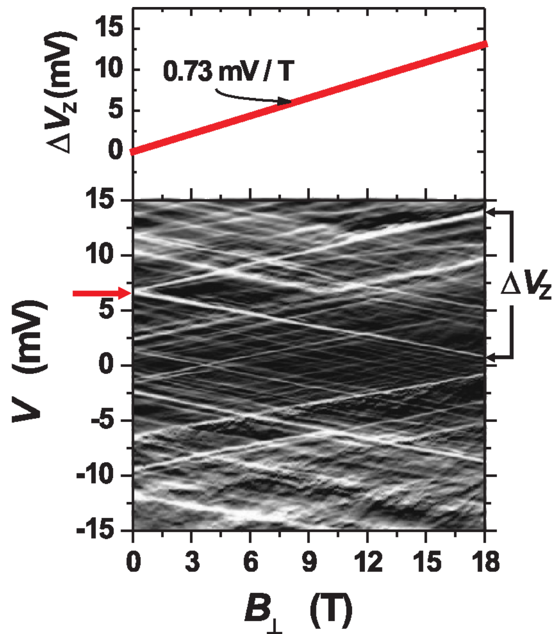

FIG. 4 (color online). Gray-scale plot of the differential conductance at 50 mK for a magnetic field orientated perpendicular to the epitaxial layer, where a dark (bright) shade corresponds to small (large) conductance. Exemplarily, the top graph shows the splitting of a level, marked by an arrow at 6.5 mV.

The giant anisotropy of the Zeeman splitting is a consequence of the effective spin $J = 3/2$ of the valence band states (Fig. 1). For a detailed interpretation of our experimental results, we have performed self-consistent calculations in the multiband envelope-function approximation [19] of the valence band profile of the active region using the nominal growth parameters. The results of the calculation are plotted in Fig. 2(b). The solid (dashed) lines show the HH (LH) subbands and the strain-split effective potentials for these states. The calculation predicts a splitting of the lowest HH and LH subbands of about 200 meV. This huge HH-LH splitting is caused by the strong quantum confinement of the thin Ge layer and the large biaxial strain due to the lattice mismatch between Ge and Si. Furthermore, the calculations support the assumption that for small applied voltages only HH states participate in transport because LH states in the SiGe and Ge QWs get occupied only at significantly higher voltages.

The behavior of the HH states in our device is in sharp contrast to electron states for which it is well-known that the Zeeman splitting is proportional to the total magnetic field B irrespective of the orientation of B relative to the epitaxial layer. Furthermore, confinement potential and strain do not affect the Zeeman energy of electron states. In the case of HH states, on the other hand, the Zeeman splitting in a field $B_\parallel$ competes with HH-LH splitting; Zeeman splitting is smaller the larger the HH-LH splitting and vice versa [19]. The appropriate situation can be created in a narrow QW or by application of uniaxial or biaxial stress. Our samples satisfy both of these requirements so that we obtain a huge HH-LH splitting, as can be seen in the band profile in Fig. 2(b), resulting in a vanishingly small Zeeman splitting in a field $B_\parallel$. This explains why we do not observe a Zeeman splitting in Fig. 5.

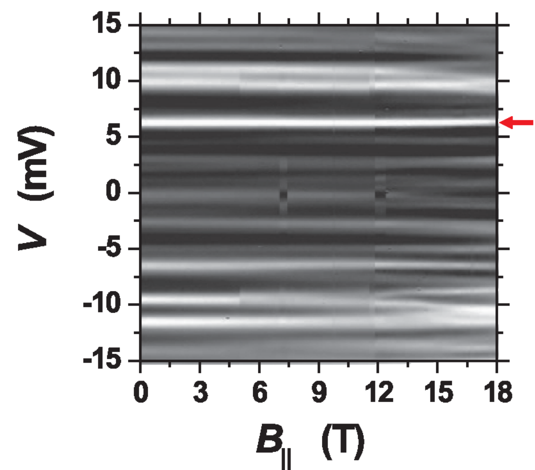

FIG. 5 (color online). Gray-scale plot of the differential conductance at 1 K for a magnetic field orientated parallel to the epitaxial layer, where a dark (bright) shade corresponds to small (large) conductance. The arrow on the right points to the same level as in Fig. 4.

In the discussion of Fig. 1 only the isotropic part of the bulk Zeeman term was taken into account [18,19]. This is the dominant term. The anisotropic part is typically 2 orders of magnitude smaller than the isotropic part and the calculations predict for our structure that it gives rise to a linear splitting with $\Delta E_{\mathrm{HH}}^{\parallel} \approx 0.18$ meV at $B_{\parallel} = 18$ T. Such a small splitting cannot be resolved in our experiment due to the width of the conductance peaks. It corresponds to $g_{\mathrm{HH}}^{\parallel} \approx 0.17$ which is almost 2 orders of magnitude smaller than $g_{\mathrm{HH}}^{\perp} = 6.3$.

In rare cases of conductance peaks we see a slightly different behavior. In Fig. 5 two conductance maxima at $+10$ and -10 mV indicate a small nonlinear splitting above 10 T. If HH-LH coupling is taken into account, we get a splitting cubic in $B_{\parallel}$ and inversely proportional to the HH-LH splitting, $\Delta E_Z \propto B_{\parallel}^3/|E_{\mathrm{HH}} - E_{\mathrm{LH}}|$ (Ref. [19]). For a fully strained system [Fig. 2(b)] the calculated splitting due to this term is even smaller than the splitting due to the anisotropic Zeeman term. However, it is conceivable that the levels showing a splitting nonlinear in $B_{\parallel}$ are related to shallow acceptors situated in sample regions of slightly relaxed strain (e.g., close to misfit dislocations). In these regions the HH-LH splitting is thus reduced and the cubic Zeeman splitting increases for these levels. This can explain why a nonlinear splitting is observable for the two conductance peaks at ± 10 mV, but not for the majority of the conductance resonances which are due to impurities in highly strained regions.

In conclusion, we have performed a detailed study of Zeeman splitting of shallow acceptor levels in a thin Si/Ge/Si quantum well, by using resonant-tunneling spectroscopy. In a magnetic field orientated perpendicular to the layer a large linear Zeeman splitting can be observed for magnetic fields up to 18 T. In an in-plane magnetic field the Zeeman splitting is suppressed. The giant anisotropy of the Zeeman splitting is a consequence of the huge heavy-hole–light-hole splitting produced by a large biaxial strain and a strong quantum confinement in the narrow Ge quantum well. It opens a new way to g-factor engineering for spintronics and quantum computing.

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