Direct observation by resonant tunneling of the B\(^+\) level in a delta-doped silicon barrier

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We observe a resonance in the conductance of silicon tunneling devices with a \(\delta\)−doped barrier. The position of the resonance indicates that it arises from tunneling through the B\(^+\) state of the boron atoms of the \(\delta\)−layer. Since the emitter Fermi level in our devices is a field-independent reference energy, we are able to directly observe the diamagnetic shift of the B\(^+\) level. This is contrary to the situation in magneto-optical spectroscopy, where the shift is absorbed in the measured ionization energy.

The smallest semiconductor device with potential functionality is a semiconductor nanostructure with a single dopant atom. The properties of such a structure are most prominent at low temperature, where the electron or hole is localized at the parent donor or acceptor, respectively. Manipulation of the wave function of the charge carrier at the dopant atom with the electric field of a gate is the obvious tool to influence the properties of the nanostructure. A good first order description of the properties of dopant atoms is given by the hydrogen model. The resulting Bohr radius of up to about 10 nm sets the size of a dopant atom and thus of a single-dopant-atom functional device. This radius is much larger than for the hydrogen atom, due to scaling for the effective mass of the carrier and the dielectric constant of the semiconductor. Such dimensions are accessible with e-beam lithography and scanning probe techniques. This opens the way for what can be called atomic scale electronics inside a semiconductor. Silicon is very attractive for this purpose because of its highly developed fabrication technology.

A beautiful example of atomic scale electronics inside silicon is the quantum computer proposed by Kane\(^1\) and by Skinner et al.\(^2\). Both the fabrication and electrical operation of the qubits of this computer rely on control at the level of individual phosphorus donors. The highly controlled dopant engineering required for atomic scale electronics inside silicon is being worked on by several groups\(^3,4\). Doping at the atomic scale for application purposes is thought to be feasible, but development of this technique will be time consuming.

A more direct way to a single dopant atom in silicon, albeit less controlled concerning exact positioning, is to use \(\delta\)−doping and conventional nanostructuring. Single-dopant-atom structures fabricated in this way will yield physics relevant for future devices fabricated with atomic scale doping techniques. To some extent this approach has been followed already, by including a \(\delta\)−layer of dopant atoms in the well of double barrier diodes\(^5\). Here, we report a transport study on \(\delta\)−doped silicon tunneling devices grown with a single barrier. The dopant atoms induce zero-dimensional atomic quantum wells, giving many identical double barrier systems in parallel. This device, a precursor of a single-dopant-atom device of a geometry close to a qubit of Kane’s computer, shows very interesting transport properties. In particular, we find a conductance resonance due to tunneling through the boron impurities of the \(\delta\)−layer in the barrier. The position of the resonance and its magnetic field dependence indicate that it originates from tunneling through the B\(^+\) state of the boron impurities. So far, this state has only been observed in spectroscopic studies using photons or phonons and not in an energy resolved transport experiment like ours.

We fabricate the \(\delta\)−doped devices from a layered structure of the type p\(^+\) Si(500 nm)/p\(^−\) Si(20 nm)/\(\delta\)/p\(^−\) Si(20 nm)/p\(^+\) Si(500 nm). Boron is the dopant, for the layers and the \(\delta\)−spike. The structure is deposited by chemical vapor deposition in an ASM Epsilon 2000 reactor on a Si(001) substrate with low doping, using SiH\(_4\) and B\(_2\)H\(_6\) as precursor gases. The \(\delta\)−spike of areal density 1.7 \(\times\) 10\(^{11}\) cm\(^−2\) is centered in the lowly doped 40 nm thick tunnel barrier. The p\(^+\) layers are degenerately doped (\(N_B = 10^{19}\) cm\(^−3\)) and serve as contact layers. The devices are square mesas, 100, 200, 300 and 400 \(\mu\)m at a side. They are dry-etched in an SF\(_6\) plasma. The etch mask is the Al-1%Si top contact of the mesa, which is sputter-deposited through a shadow mask. The SF\(_6\) etch is stopped just after the bottom p\(^+\) layer has been reached. A second shadow mask, aligned with respect to the mesas, is used for sputter deposition of Al-1%Si contacts to the bottom layer. The final step is a 400 °C anneal in N\(_2\)/H\(_2\) of the Al contacts to the p\(^+\) Si, using rapid thermal processing. A high device quality is apparent from resistance scaling with mesa size. At room temperature the resistance is dominated by the two-dimensional spreading resistance of the bottom layer between the mesa and the Al contact, while at low temperature it is determined by the barrier in the mesa. These devices, which have a metal-insulator-metal structure, are the simplest all-silicon tunneling devices.

We measured the doping profile in the structure with secondary ion mass spectroscopy (SIMS). Figure II(a)
The top layer is only 20 nm thick. Contact layers, barrier and δ-layer are clearly visible. (b) Depicts the profile of the valence-band edge, the hole energy increasing in the upward direction. Fermi seas of emitter and collector extend up to the barrier, of which the thickness is defined with the criterion $N_B = 4 \times 10^{18} \text{ cm}^{-3}$, the concentration of the metal-insulator transition. Symbols are discussed in the text.

Figure 1: (a) SIMS profile of the boron concentration. Zero depth is the surface position. For optimum resolution the top layer is only 20 nm thick. Contact layers, barrier and δ-layer are clearly visible. (b) Depicts the profile of the valence-band edge, the hole energy increasing in the upward direction. Fermi seas of emitter and collector extend up to the barrier, of which the thickness is defined with the criterion $N_B = 4 \times 10^{18} \text{ cm}^{-3}$, the concentration of the metal-insulator transition. Symbols are discussed in the text.

Figure 2: Conductance curves of 400 μm device 1/888/1, for the temperatures listed. With decreasing temperature the conductance decreases (for the lower temperatures most clear at higher biases) and a resonance at ±10 mV develops. Between 1.5 and 0.5 K the resonance still grows.

The conductance peak is attributed to resonant tunneling through the B\textsuperscript{+} state of boron impurities in the δ-layer, each of which provides for a conductance channel. The B\textsuperscript{+} state is an acceptor counterpart of the more generally known D\textsuperscript{−} state. It forms when a second hole is weakly bound to a neutral acceptor, in our case neutral boron B\textsuperscript{0}. In zero magnetic field the B\textsuperscript{+} state is a singlet state (as the D\textsuperscript{−} state is), which is analogous to the negative hydrogen ion (H\textsuperscript{−} ion). The separation of the B\textsuperscript{0} ground-state level and the B\textsuperscript{+} level results from the Coulomb interaction between the holes. In our devices the B\textsuperscript{0} ground state is deep below the Fermi level, so that it is permanently occupied. Therefore, higher levels of the B\textsuperscript{0} single hole spectrum are not available as stepping stones for holes tunneling from emitter to collector. This means that the B\textsuperscript{+} state is the only candidate which can induce the resonance. This is unlike an optical absorption experiment in which higher levels may always come into play via transitions from the ground state.

From photoconductance spectroscopy on Si samples with low doping level it is known\textsuperscript{10} that in zero magnetic field the binding energy $E^+(0)$ of the extra hole on an isolated B\textsuperscript{+} ion, i.e. the amount of energy required to
remove this hole from the ion to the valence band edge, is about 2.0 meV. This is close to 0.055 Ry* = 2.5 meV predicted by the H− ion model, which is successfully used for the D− state. Here Ry* is the effective Rydberg for boron in silicon, which equals the ground state energy \( E_1 = 45.7 \text{ meV} \). Since the measured resonance comes from the \( \delta \) layer, equal parts of the bias drop across the barriers at either side of the Coulombic potential well associated with a boron impurity. Thus, the resonance voltage is \( V_{\text{res}} = 2(\phi_B - E^+(0))/e \) [see Fig. 1(b)]. We determine \( \phi_B \) from the temperature dependence of the zero-bias resistance \( R_0 \). When plotted versus \( 1/T \), the logarithm \( \ln(T^2 R_0) \) clearly shows activated behaviour in the range 15-20 K. Interpreting this as Richardson-Dushman thermionic emission \( \text{of holes over the barrier} \), we find \( \phi_B = 11.7 \text{ meV} \) from a fit to the data. This is not too far from \( \phi_B = \Delta E_0 - E_F = 8 \text{ meV} \) which we obtain from the estimate \( \Delta E_0 \) for \( \Delta E_0(N_B) \) and from photoluminescence measurements \( E_F(N_B) \), each subject to uncertainty. The values \( \phi_B = 11.7 \text{ meV} \) and \( E^+(0) = 2.0 \text{ meV} \) predict \( V_{\text{res}} = 19.4 \text{ mV} \). This deviates strongly from the measured position and thus seems to exclude the \( \delta^+ \) state. However, the concentration \( N_B = 5 \times 10^{17} \text{ cm}^{-3} \) of the \( \delta \)-layer is high enough for the tail of the wave function of the second hole to be appreciable at the nearest \( B^0 \) atoms, so that the \( \delta^+ \) ions are not isolated. The additional Coulomb attraction of these \( B^0 \) atoms and spreading of the electron charge among them (reducing the hole-hole repulsion at the \( \delta^+ \) state) cause a stronger binding. This effect increases with increasing concentration. The measured \( V_{\text{res}} \approx 10 \text{ mV} \) gives \( E^+(0) \approx 6.7 \text{ meV} \). As demonstrated in Fig. 4, this value nicely falls in the bandwidth obtained by extrapolating the scarce experimental data \( 14, 15, 16 \) on the concentration dependence of the ionization energy for \( \delta^+ \) and \( \delta^- \).

In the lower part of the temperature range of Fig. 2 the resonance is much wider than the theoretical width \( 3.5kT \) of a Fermi-smeared sharp resonance, implying a rather large zero temperature width (\( \approx 1.5 \text{ meV} \)). Mechanisms contributing to this are lifetime broadening, disorder broadening and broadening due to the finite width of the \( \delta \)-layer. Life-time broadening determines the intrinsic width of a resonance coming from a single impurity. For the \( \delta^+ \) level lifetime broadening is appreciable, since it is so close to the ionization level. The effect is enhanced by the large bias field at resonance (2.5 kV/cm), which weakens the collector barrier and thus shortens the lifetime. We will come back to this in discussing broadening of the resonance with increasing magnetic field (see below). Disorder broadening arises from the different local surrounding of \( B^0 \) centers by adjacent \( B^0 \) centers, which causes a distribution of levels. The finite width of the \( \delta \)-layer implies a range of values of \( V_{\text{res}} \), since the position of the atom defines the barrier thicknesses and thus the distribution of the bias over them. Without correcting for a decay of the resonance for off-center position \( 17 \), a range for \( V_{\text{res}} \) of 3.5 meV is derived from only the finite \( \delta \)-layer width. We take this as a sign that the \( \delta \)-layer width is an important source of broadening.

The resonance shift to higher bias (Fig. 3) reflects the diamagnetic shift \( \Delta E_{\text{dia}}(B) \) of the \( \delta^+ \) level in a magnetic field. This shift, termed diamagnetic because of the related negative susceptibility, is towards the valence band edge, in agreement with the observed peak shift to higher biases. In magneto-optical spectroscopy the diamagnetic shift is not obtained directly, since it is absorbed in the field-dependent binding energy \( E^+(B) = E^+(0) + \frac{\hbar}{2} \omega - \Delta E_{\text{dia}}(B) \). Here \( \frac{\hbar}{2} \omega \) is the energy of the first Landau level, which is the valence-band edge in field. In our experiment, however, since the emitter doping level \( N_B = 10^{19} \text{ cm}^{-3} \) is high enough to block Landau level formation in this layer, the emitter Fermi level is a field-independent reference energy enabling direct mea-
measurement of $\Delta E_{\text{dia}}(B)$. For the weak fields used here, first order perturbation theory estimates the diamagnetic shift as

$$\Delta E_{\text{dia}}(B) = \frac{e^2 B^2}{12 m} \sum_{i} r_i^2.$$  

Here $m$ is the effective mass of the holes of the $B^+$ ion and $r_i^2$ is the mean square distance of the $i$-th hole to the $B^+$ core ($i = 1, 2$). Taking $m_{a0} = 0.15 m_0$ and $m_{hh} = 0.54 m_0$ for the light and heavy hole mass, respectively, and $r_i^2 = a_i^2$ for the first hole ($a_0 = 3.9$ nm is the Bohr radius of the $B^0$ atom), we fit the expression for $\Delta E_{\text{dia}}(B)$ to the complete set of data points of Fig. 3. This yields the fit shown in the figure and corresponding values $r_1^2 = (1.6 a_0)^2$ and $r_2^2 = (3.4 a_0)^2$. The range defined by these values is consistent with $r_2 = 2.4 a_0$ cited for the $B^+$ state. We attribute the deviation of the fitted curve from the experimental trend to the use of an atomic physics model for $\Delta E_{\text{dia}}$ in a solid state system.

Broadening of the resonance with increasing magnetic field may be unresolved splitting and/or life-time broadening induced by the Stark effect. Since the resonance voltage increases with increasing magnetic field, the electric field at resonance, and thus the Stark broadening, increase as well. Data for Stark broadening of the $B^+$ level are not available. Therefore, we take as a measure the broadening of the far infrared absorption line due to transition from the ground state of $B^0$ atom in silicon to the first excited state, which was measured up to 1.0 kV/cm. Extrapolation of the data of Ref. [21] to the fields of our experiments yields an increase of the halfwidth between 0 T and 14 T of 0.1 meV, to be compared with our measured increase of 0.5 meV. Stark broadening apparently plays a role.

Finally, we discuss the background contribution to the conductance (see Fig. 2), which shows a weak temperature dependence below 4.2 K. The parabolic shape of the background suggests direct tunneling as transport mechanism. However, the conductance at $V = 0$ is several orders of magnitude higher than expected for direct tunneling, so that it is excluded. Hence, the background conductance is due to hopping resulting from the background doping in the barrier. This hopping is thermally activated close to $V = 0$ and field activated at higher biases ($|V| \geq 2$ mV). For biases exceeding the barrier height ($|V| \geq 11.7$ mV), the barrier becomes increasingly weak for hopping and finally for direct tunneling, giving a further conductance increase. Above 4.2 K the conductance in the range ($|V| \leq 2$ mV) undergoes a transition to coexistence of thermal hopping and thermal activation over the barrier and finally to dominance of activation over the barrier.

In conclusion, we have studied resonant tunneling through a Si barrier $\delta$–doped with boron impurities. The conductance resonance observed is due to tunneling through the $B^+$ state of the impurities. The structure of our device enables direct observation of the diamagnetic shift of the $B^+$ state. The measured magnitude of the shift agrees well with the theoretical description, yielding a proper value of the orbit size for the second hole of the $B^+$ state. The binding energy of the $B^+$ state turns out to be enhanced as a result of overlap of the wave function of the second hole of the $B^+$ state with the nearest boron impurities. Our next step will be miniaturizing the devices to the level of one dopant atom (diameter$\approx 50$ nm), enabling studies of the effect of wave-function manipulation on transport through the atom.

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