Conduction band discontinuity and electron confinement at the Si_xGe_{1-x}/Ge interface

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Germanium rich heterostructures can constitute a valid alternative to Silicon for the confinement of single electron spins. The conduction band discontinuity in SiGe/Ge heterostructures grown on pure germanium substrate is predicted to allow the confinement of electrons in the germanium, and the conduction band profile of germanium rich heterostructures allow the implementation of *g*-factor modulation devices not possible in Silicon. We here prove that electrons can indeed be trapped at the $Si_{0.1}Ge_{0.9}$/Ge interface and we measure the height of the energy barrier to 0.55 ± 0.05 eV by measuring the tunneling time of electrons as a function of the electric field. © *2010 American Institute of Physics*. [doi:10.1063/1.3432066]

Single electron devices can be efficiently realized on Silicon substrates, where either metal oxide semiconductor like structures or Si/SiGe strained quantum wells[1,2] are used to confine electrons in the growth direction, and electrostatic gates are used for the in-plane confinement. While electrons in germanium also have long electron spin coherence time and heterostructures for electron confinement are possible, devices based on this material remain mostly unexplored. A type I band alignment is predicted[3,4] from theoretical calculation for $Si_{1-x}Ge_x$ epilayers grown on pure germanium when Silicon concentration is less than about 30%. Germanium has the conduction band (CB) minimum in the (111) crystallographic direction, while SiGe epilayers, due to the stress consequence of the lattice mismatch, can have the CB minimum in either (111) or (100) direction, if the silicon content is less or more than 10%–15%. These properties can be exploited in devices using *g*-factor modulation schemes, as proposed in Ref. 5 and benefiting of the total valley degeneracy lifting possible on (111) substrates.

One of the obstacles to the use of such devices is that the energy barrier available to confine electrons is limited to about 50–100 meV, as extracted from theoretical calculations:[3,4] this is consequence of the strain in the SiGe epilayer that shifts the band minima and causes the energy barrier to decrease when Silicon concentration larger than 15% is used. Besides, no experimental verification of the barrier height is available to date. In this work we want to experimentally measure the height of the CB discontinuity in a SiGe/Ge heterostructure, proving that it is possible to confine electrons at that interface, and measure how long electrons can be confined before tunneling occurs.

The heterostructure used in this work was grown with a home-built ultra high vacuum CVD system on a π-Ge (100) (10 Ω cm) substrate. On top of that, a 200 nm thick p^+ layer, with Boron concentration of 2 10^{18} cm^{-3}, a nonintentionally doped Ge layer 900 nm thick and a 30 nm $Si_{0.11}Ge_{0.89}$ barrier were grown. The barrier thickness and alloy were verified by transmission electron microscopy and secondary ion mass spectroscopy, respectively. These values are well below the Matthews and Blakeslee stability limit so that no strain relaxation is expected. On this substrate we fabricated a Schottky diode as shown in Fig. 1(a), using semitransparent titanium for the blocking contact. Notoriously the metal Fermi level is pinned close to the germanium valence band,[6] so that even at liquid helium temperature most metals tested, such as nickel, platinum, and aluminum gave quasi Ohmic I-V characteristics. Only titanium reliably formed a good Schottky barrier with a reverse leakage current limited to 10^{-8} A/cm^2 up to 1 V bias. The back contact was realized etching the spacer down to the p^+ layer and depositing aluminum subsequently annealed at 400 °C. The device area was limited to 100×100 μm^2 to ensure uniformity of the barrier.

As evidenced in Fig. 1(b), when the device is reverse biased, a triangular quantum well for electrons is formed

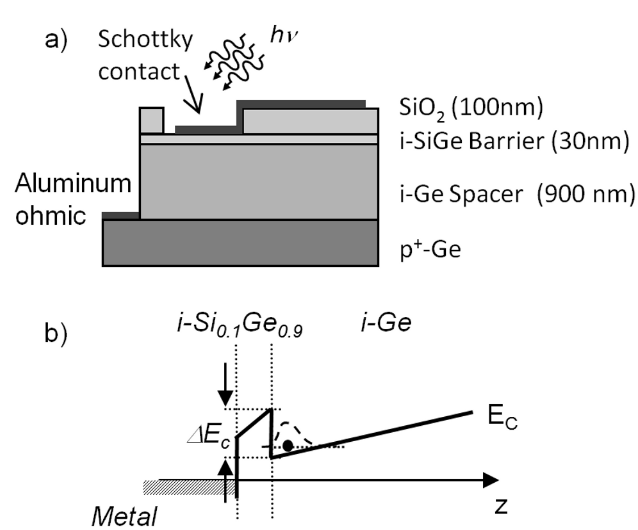

FIG. 1. (a) Schematic cross-section of the heterostructure and Schottky diode used in the work (b) detail of the triangular potential well formed under the SiGe/Ge interface.

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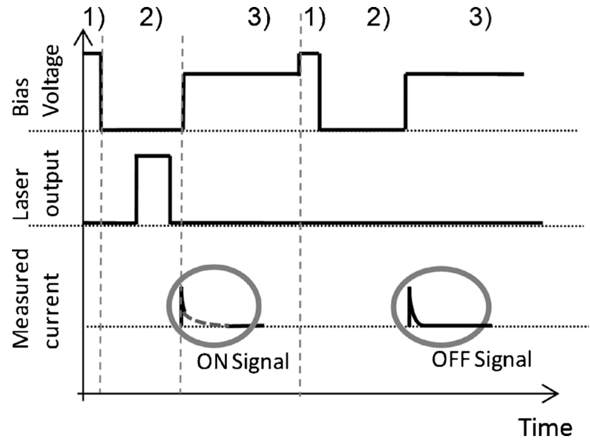

FIG. 2. Schematic time diagram of the measurement sequence of the (from top to bottom) bias voltage, illumination, and device current during the measurement. Steps from 1 to 3 are repeated twice, but only during the first iteration the laser is turned on. The current diagram schematically shows the capacitance charging current with the additional long tail observed when confined electrons are accumulated.

under the SiGe/Ge interface, delimited at the left (top) side by a trapezoidal barrier. Being the barrier height in the 50–100 meV range and the thickness limited to few tens of nanometers, a considerable tunneling probability is expected.

Experiments were performed in liquid helium, to eliminate any thermally activated process. To detect the trapping and tunneling of electrons through the barrier we photogenerated electron-hole pairs by absorption of a 630 nm radiation: the internal electric filed is such that holes are collected at the substrate while electrons accumulate under the barrier and eventually tunnel through it and are collected at the Schottky contact. After the photogeneration electron tunneling is detected by measuring the current flowing through the device. Electrons tunneling through the barrier induce a charge on the electrodes equivalent to that generated by a charge moving inside the plates of a capacitor. In our device each electron induces a total charge equivalent to $t_b/(t_b+t_s)\cdot q \simeq 0.03\cdot q$, where t_b and t_s are the thicknesses of the barrier and spacer, respectively, and q is the electron charge.

In order to maximize the available signal electrons were generated at zero bias, where tunneling is slower and a higher electron density can be obtained; detection was then performed at a larger reverse bias, to increase the tunneling probability, and therefore, the current signal. Each measurement sequence, depicted in Fig. 2, consists of three steps:

(1) A large reverse bias peak is applied to the junction in order to remove any electrons possibly present at the interface.
(2) The bias is set to 0 V and a light pulse is sent to photogenerate the electrons.
(3) The bias voltage is increased again and the photocurrent is measured: the voltage applied in this phase, referred to as the extraction voltage, is used to control the tunneling probability.

Charging the total device capacitance of 3 pF at the beginning of the third step requires a charge at least one order of magnitude larger than that induced by the electrons tunneling. To discriminate the two contributions the previous bias sequence is repeated two times, where, at the second iteration, no light pulse is applied. The two current signals measured at each iteration are subtracted to each other and numerically integrated to obtain the charge signal generated by the tunneling of the trapped electrons.

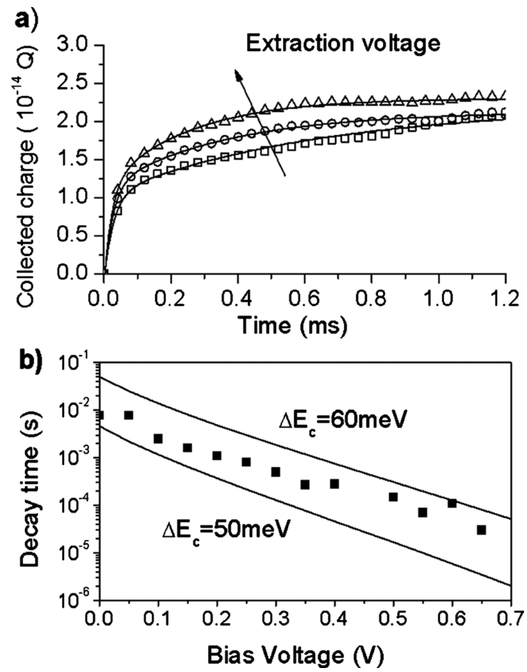

FIG. 3. (a) Time traces of the collected charge at extraction voltages of 0.3, 0.35, and 0.4 V. Symbols are experimental data and lines are the best fitting two-exponential curves. (b) Decay time of the electron density vs the bias voltage. Dots are experimental data while the two lines are calculated for barrier heights of 50 and 60 meV.

Figure 3(a) shows typical charge versus time signals recorded at three different extraction voltages, where the origin of the time scale is set at the beginning of the third voltage step. The experimental data are fit with a two exponential decay curve. The faster exponential has time constant limited by the amplifier bandwidth, 50 kHz for the traces reported, and amplitude proportional to the change of bias voltage at the beginning of the third step: we attribute this signal to a relatively small modification of the total device capacitance consequence of light absorption.

Conversely, the charge collected with a slower time constant can be attributed to electrons tunneling through the barrier. As expected, the risetime, corresponding to the average tunneling time, is strongly dependent on the applied bias, while the total collected charge is constant at $10^{-14}\pm 0.1\times 10^{-14} Q$, corresponding to a density of trapped electron of 2×10^{-10} e^-/cm^2. The tunneling times obtained as a function of the extraction voltage are reported as the full markers in Fig. 3(b).

To confirm the validity of the experiments and extract the effective height of the tunneling barrier we developed a semiclassical model to calculate the electrons tunneling time. In this model we used the physical dimensions measured for the device previously characterized, so that the only free parameter left is the energy barrier height at the SiGe/Ge interface.

The average tunneling time is $\tau_t = \Theta/\nu_e$, where Θ is the tunneling probability and ν_e the attempt to escape frequency. The tunneling probability for a trapezoidal barrier calculated through the Wentzel-Kramers-Brillouin (WKB) approximation is, as follows:[7]

$$\Theta = \exp\left\{ -\frac{4}{3}\sqrt{\frac{2m^*}{\hbar^2}}\frac{1}{qE_b}[(\Delta E_c - E_0)^{3/2} - (\Delta E_c - E_0 - qE_b t_b)^{3/2}]\right\},$$

where ΔE_c is the CB discontinuity, E_0 the kinetic energy of the electron in the triangular well, E_b the electric field in the barrier, t_b the barrier thickness, and $m^*=0.12\times m_0$ the electron effective mass in germanium.

The attempt to escape frequency can be written as the inverse of the roundtrip time of the electron inside the triangular well: $\nu_e=\sqrt{(2E_0q/m^*m_0)}(1/2w)$ with $E_0 = 2.34\{[(qE_b\hbar)^2/2m^*m_0]\}^{2/3}$.

While τ_t is generally dependent on the electron density, for values below approximately $10^{10}\ e^-/cm^2$ the dependency is slow and the decay of the electron density can be approximated as exponential. The predicted decay times for a CB discontinuity of 50 and 60 meV are reported as the continuous lines in Fig. 3(b). The experimental data are in good agreement with the model and allow extracting a value of CB discontinuity of 0.55 ± 0.05 eV, compatible with the theoretical values reported in literature. Besides, the total charge collected experimentally is in good agreement with the limit set for exponential decay of the carrier density.

Concluding, we have proven the possibility to confine electrons in germanium rich Si_xGe_{1-x}/Ge heterostructures. The trapping of electrons at the heterointerface has been experimentally measured detecting the tunneling of photogenerated electrons through the barrier. Experiments show a confinement time dependent on the applied bias voltage, as expected by the device model, with a maximum confinement time of 10 ms. Calculating the tunneling time with a semiclassical model and comparing the predicted tunneling times with the experimental ones, we could evaluate the CB discontinuity at the interface of $Si_{0.11}Ge_{0.89}/Ge$, obtaining a value of $\Delta E_C=0.55\pm0.05$ eV.

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