

# Confinement levels in SiGe quantum wells studied by charge spectroscopy

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Quantum confinement levels in SiGe quantum wells (QW) with different Ge contents were observed by means of charge deep-level transient spectroscopy (Q-DLTS) and transport measurements in the temperature range from 80 to 300 K. This turns out to be possible due to a passivation of structure surface with an organic monolayer. The confined levels became apparent through DLTS measurements as various acti-

vation energies in temperature dependence of the rate of carrier emission from the QW. It was found that the recharging of SiGe QWs and carrier emission accomplish due to thermally stimulated tunneling. The steps in the current-voltage characteristics originated from direct tunneling via the confined states were found to determine the current flow at high fields.

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**1 Introduction** The main problem in studies of Si/SiGe/Si quantum well structures with low doping level is the relatively small thickness of cap Si layer. Due to residual positive charge at surface states, the near-surface layers including the SiGe quantum well are depleted resulting in low population of the QW [1, 2]. To diminish the surface charge, it was suggested to use a passivation of Si cap layer surface by an organic monolayer deposition [3]. In this report we present the results of Q-DLTS measurements on passivated Si/SiGe/Si heterostructures with different Ge contents in QWs, as well as transport measurements, which directly indicate the emission of carriers from ground and excited confined levels in QWs.

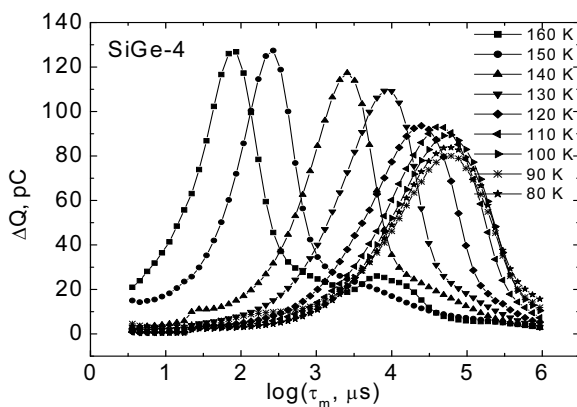
**2 Experimental** The Si/SiGe/Si structures with different Ge fractions  $x$  in the SiGe layers, designated below as SiGe-1, SiGe-2, SiGe-3 and SiGe-4 for  $x = 0.07, 0.10, 0.15,$  and  $0.25,$  respectively, have been used in the present study. The structures were grown by molecular beam epitaxy (MBE) on n-type float-zone Si substrates at the tem-

perature of 400 °C. The SiGe layer of 14 nm thickness was  $\delta$ -doped in the middle with boron at a concentration of  $6 \times 10^{11} \text{ cm}^{-2}$ . Two B  $\delta$ -layers with the same concentration were positioned within the buffer and cap layers (one each). The thicknesses of the buffer and cap layers were 80 and 38 nm, respectively. To provide low surface charge and high carrier concentration in the SiGe quantum wells, the surface was passivated with organic monolayer of 1-octadecene [3]. The passivated samples were characterized by high-frequency (1 MHz) capacitance-voltage (CV) and vertical (across the layers) current-voltage (I-V) characteristics in dependence on temperature, as well as by charge deep-level transient spectroscopy (Q-DLTS). A mercury probe and Ag electrodes deposited on the surface were used as electric contacts. The system employed in the present work for measurements of Q-DLTS spectra kept the sample temperature fixed and scanned the rate window  $\tau_m$ , where  $\tau_m = (t_2 - t_1) / \ln(t_2/t_1)$ ,  $t_1$  and  $t_2$  are the time moments of recording the Q-DLTS signal  $\Delta Q = Q(t_2) - Q(t_1)$ . According to the theory, the emission rate of carriers from the QW

can be described as  $e_T \sim T^{1/2} \exp(-E_a/kT)$  [4, 5],  $E_a$  is the activation energy.

**3 Results and discussion** The Si/SiGe/Si structures with different Ge fraction in SiGe alloy were studied by Q-DLTS. Typical Q-DLTS spectra are given in Fig. 1 for structure SiGe-4. The position of maximum in the spectrum changed with the temperature and demonstrated the activation behavior. Note that this maximum was observed only in the passivated structures. We attribute the origin of this peak to the carrier emission from confined levels in the SiGe QW.

The  $\tau_m$  value of a peak position in Q-DLTS spectra gives directly the characteristic time of discharging corresponding electronic state. With decreasing temperature from 220 K to 100 K, the characteristic time for emission of carrier from the levels in QW changed from 10 to 100  $\mu$ s for SiGe-1, SiGe-2 and SiGe-3. For higher Ge content (SiGe-4) the characteristic time increased up to 0.1-100 ms. Fig. 2 shows Arrhenius plots for the values of  $\tau_m$  at the maximum in dependence on  $1/T$  for the structure with Ge fraction of 7%. It is possible to extract several activation energies in different temperature ranges. We have tried to find the correlation between the energies extracted from Q-DLTS data and the energies  $E_i$  of size quantization in QW calculated in [6]. However, the experimental activation energies didnot agree with the calculated energy values. It turns out that the experimental activation energies can be fit by taking into account a band bending between the QW and Si cap and buffer layers in the passivated structures, which form triangle barriers. In this case, the activation energy should be the difference between the confined state energy  $E^*$  counted from the QW bottom and some value  $E_0$  corresponding to the optimal energy of thermo-stimulated tunneling.



**Figure 1** Q-DLTS spectra for SiGe-4 structure measured at fixed filling pulse duration of  $10^6 \mu$ s at different temperatures.

The energy of optimal tunneling for a triangle barrier can be found from the maximum of the dependence of the exponential functions of thermal emission rate and tunneling probability on carrier energy  $E$ :

$$W \propto \exp\left(-\frac{E^* - E}{kT}\right) \exp\left(\frac{4\sqrt{2m}E^{3/2}}{3\hbar eF}\right), \quad (1)$$

where  $E^* = \Delta E - E_i$ ,  $\Delta E$  is the valence band offset,  $m$  is the carrier effective mass,  $e$  is the elementary charge and  $F$  is the electric field strength at the triangle barrier. The emission rate at thermally stimulated tunneling is then given by the expression (cf., e.g., (10.21) in Ref. [7])

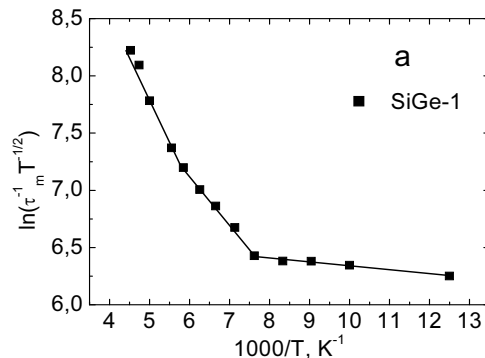
$$e_r(F) = \exp\left[-\frac{E^*}{kT} + \frac{1}{6mkT} \left(\frac{eF\hbar}{2kT}\right)^2\right] = \exp\left[-\frac{1}{kT}(E^* - E_{or})\right], \quad (2)$$

where

$$E_{or} = \frac{1}{6m} \left(\frac{eF\hbar}{2kT}\right)^2$$

is the lowering of potential barrier due to tunneling. The experimental values of  $E_0$  are in reasonable agreement with Equation (2); in particular,  $E_0$  obeys the expected  $T^{-2}$  dependence [6].

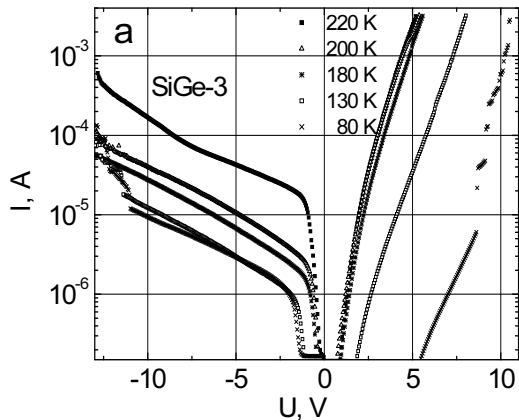
Thus, the high population of SiGe QW, which was obtained by means of surface passivation, allowed us to observe confined levels at relatively high temperatures (above the temperature of liquid nitrogen) during the recharging of QW that is a transient process. We will show now that the QW confined states can be evident at the stationary conditions.



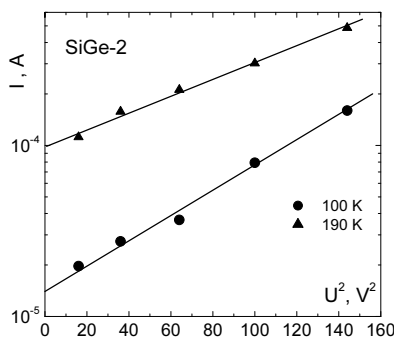
**Figure 2** Arrhenius plots of log rate window time versus reciprocal temperature for structure SiGe-1 in the temperature range from 80 to 300 K. Duration of filling pulse was 1 s.

In Fig. 3 the vertical I-V characteristics of the passivated Si/SiGe/Si structures are presented, which were found to be transistor-like. That is the result of Schottky barrier on the surface connected in series with p-n junction between p-Si layers with SiGe QW and n-Si substrate. In both polarities, the exponential growth of current at low voltages is the result of tunneling carriers through a triangle barrier at the surface formed due to Shottki contact. To prove this, we analyzed the same Eq. (2). The energy of optimal thermo-stimulated tunneling is proportional to  $F^2$ . Shown in Fig. 4 is the dependence of the current through the sample on voltage in the scale  $(\log I - U^2)$  for negative

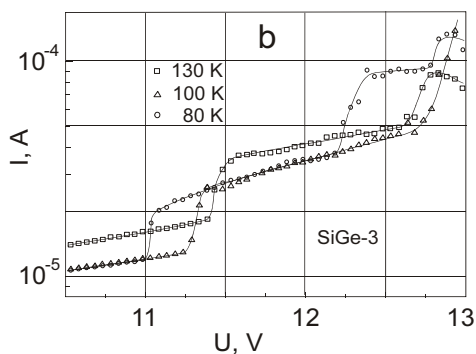
polarity (blocked p-n junction). It is seen that this dependence gives very good fit to the experiment.



**Figure 3** Current-voltage characteristics of passivated SiGe-3 structure for different temperatures.



**Figure 4** Log I plot vs  $U^2$  for negative voltage (blocked p-n junction)



**Figure 5** Current-voltage characteristics at high fields for negative applied voltage.

At voltages above  $\sim 2$ -5 V, the electric field at the triangle barrier near the surface becomes  $> 2\text{-}4 \times 10^5$  V/cm, the  $E_0$  value becomes comparable with the barrier height and at low temperatures (80-120 K) the thermo-stimulated tunneling should change for direct tunneling. In some voltage range, the tunnel transitions can pass through the QW. At

low temperatures, such transitions are possible only at the energies coincided with the energies of size quantization.

Figure 5 presents part of I-V curves at high voltages. The steps corresponding to the direct tunnel transitions via confined QW levels are clearly seen. Note that the confined levels take part in the vertical conductivity of passivated SiGe/Si structures at the temperatures below 130 K as opposed to the case of QW recharging observed in DLTS measurements up to T near the room temperature. At higher T the thermal excitation of carriers becomes significant masking the tunneling.

**4 Conclusions** The organic surface passivation was found to increase strongly the population of the SiGe quantum wells in single-QW Si/SiGe/Si structures. This gives the possibility to observe the system of the quantum confinement levels in SiGe QW for structures with different Ge content in SiGe alloy. The key role of thermo-stimulated tunneling in carrier emission from the QW and of direct tunneling through the confined states was ascertained.

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