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Deep-level spectroscopy studies of confinement levels in SiGe quantum wells

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The recharging of quantum confinement levels in SiGe quantum wells (QWs) was studied by charge deep-level transient spectroscopy (Q-DLTS) for Si/SiGe/Si structures with different Ge contents in the SiGe layer. The set of levels were observed as the different slopes in the Arrhenius plots for the same Q-DLTS peak in different temperature ranges. These activation energies were compared to the energies of quantum confinement levels in the QW calculated in frames of six-band model taking into account spin-orbit interaction and attributed to a thermally activated tunneling of holes from the SiGe QW. © *2009 American Institute of Physics*. [doi:10.1063/1.3153974]

I. INTRODUCTION

At present there is considerable interest in studying the electronic capture-emission properties of Si/SiGe/Si quantum well (QW) heterostructures, suitable for terahertz lasers,[1] for example. Deep-level transient spectroscopy (DLTS) is a powerful tool to probe the electronic properties of QW systems.[2] The main problem in studies of Si/SiGe/Si QW structures is the relatively small thickness of the Si cap layer. Due to residual positive charge at surface states, the near-surface layers including the SiGe QW are depleted resulting in low hole population of the QW, hysteresis in the *C-V* and *I-V* characteristics and the electric field effect (conductivity along SiGe layer increased with increasing applied transverse voltage).[2,3] To diminish the surface charge, we passivated the Si cap layer surface by an organic monolayer deposition.[4] In this report we present the results of Q-DLTS measurements on passivated Si/SiGe/Si heterostructures with different Ge contents in the QW, which directly indicated the emission of holes from ground and excited levels in the valence bands of QWs.

II. EXPERIMENTAL

The present study used three Si/SiGe/Si structures with different Ge fractions x in the $Si_{1-x}Ge_x$ layers, designated as SiGe-1, SiGe-2, and SiGe-3 for $x=0.07$, 0.10, and 0.15, respectively. The structures were grown by molecular beam epitaxy (MBE) on n-type float zone Si(100) substrates at the temperature of 400 °C. The Ge molecular beam was produced by thermal evaporation from a solid source of triple zone-refined crystalline Ge. The SiGe layers of 14 nm thickness were δ-doped in the middle with boron with a concentration of 6×10^{11} cm^{-2}. Two additional boron-doped δ-layers with the same concentration were positioned within the buffer and cap layers (one each). The thicknesses of the Si buffer and cap layers were 80 and 38 nm, respectively. The transmission electron micrograph (TEM) in Fig. 1 of structure SiGe-3 with maximal Ge content demonstrated that there are no large structural defects such as dislocations. The background concentration of holes in the MBE-grown layers did not exceed 3×10^{15} cm^{-3}. To provide low surface charge and high carrier concentration in the near-surface layers and the SiGe QWs, the surface was passivated with organic monolayers of 1-octadecene.[4]

Passivated samples were characterized by high frequency (1 MHz) capacitance-voltage (*C-V*) and Q-DLTS measurements. A mercury probe or Ag electrodes deposited on the surface were used as Schottki contacts. The Q-DLTS measuring system employed in the present work kept the sample temperature T fixed and scanned the rate window τ_m, where $\tau_m=(t_2-t_1)/\ln(t_2/t_1)$, and t_1 and t_2 are the moments of recording the Q-DLTS signal $\Delta Q=Q(t_2)-Q(t_1)$. The theory of using of DLTS measurements for QW diagnostics is given in Ref. 5. The expression

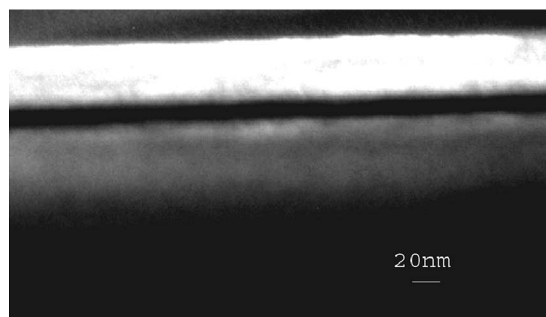

FIG. 1. Cross sectional TEM micrograph of structure SiGe-3 with maximal Ge content in the SiGe layer, showing the cap (bright upper layer), the SiGe (central dark band), and the underlying gray buffer layer and the substrate.

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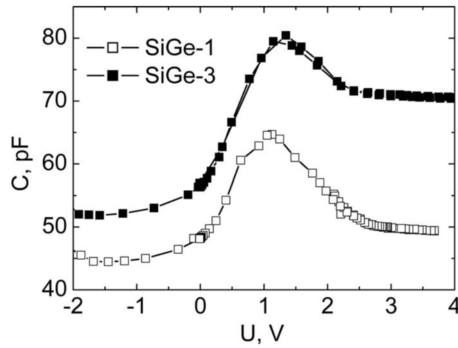

FIG. 2. Capacitance vs voltage curves for the passivated structures SiGe-1 and SiGe-3.

$$e_T \sim T^{1/2} \exp(-E_a/kT), \quad (1)$$

where E_a is the activation energy, and k is the Boltzmann constant, was used for description of the emission rate e_T of carriers from confined energy levels in the QWs.[5–7]

III. RESULTS AND DISCUSSION

The *C-V* characteristics for passivated structures SiGe-1 and SiGe-3 are given in Fig. 2. The capacitance of a Si/SiGe/Si structure includes that of the Schottky barrier on the surface connected in series with the *p-n* junction formed between the boron delta doped buffer layer and the *n*-substrate. The decrease in capacitance at negative voltages applied to the top contact was caused by depletion region formation in the substrate. Positive applied voltage corresponds to a forward bias for the *p-n* junction, and at voltage $V>1$ V the *p-n* junction capacitance becomes high enough giving a small contribution to the total series capacitance. The decrease in capacitance at positive voltages corresponds to the depletion of the epitaxial *p*-Si with SiGe layers. This diminution of capacitance at positive voltages caused by an increase in hole concentration in the near-surface layers was observed only after passivation. The *C-V* characteristics were used to optimize the voltage range for Q-DLTS measurements. For the diagnostics of the near-surface layer with SiGe QWs, we used 3 V as the constant voltage applied to the structure and −1 V for magnitude of the filling pulse.

The Q-DLTS spectra for structure SiGe-2 are given in Fig. 3(a). The position of the main peak A in the spectra changed with the temperature and demonstrated the activation behavior. Note that peak A was observed only in the passivated structures, there was no peak A before surface passivation (with native oxide on the surface). We will argue that the origin of peak A is the carrier emission from confined levels in the SiGe QW. One more peak B in the Q-DLTS spectra connected with interface defects appeared only at short enough filling pulse at $\tau \leq 10^4$ μs; it was observed for nonpassivated structures too (for details, see Ref. 2). The amplitude of peak B increased with decreasing filling pulse duration, whereas amplitude of peak A in structure SiGe-1 does not depend significantly on filling pulse duration [Fig. 3(b)]. For SiGe QW structures with higher Ge content, amplitude and position of peak A weakly changed with variation of the filling pulse duration [Fig. 3(b)]. The

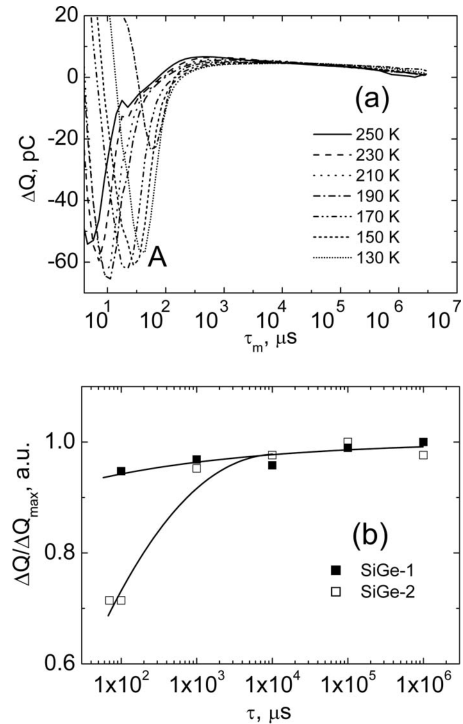

FIG. 3. Q-DLTS spectra (a) for SiGe-2 structure measured for fixed filling pulse duration of 10^6 μs at different temperatures, and the dependence of the amplitude of peak A (b) on the duration of the filling pulse τ at 80 K. Voltage applied was 3 V and magnitude of filling pulse was −1 V.

activation energy of peak B increased with Ge content in the SiGe alloy: it was 0.18 eV for SiGe-1 structure (with the carrier capture cross section of 4×10^{-15} cm^2) and 0.27 eV for SiGe-3 structure with $x=0.15$.

The τ_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 to 100 K, the characteristic time for peak A changed from 20 to 100 μs for SiGe-1, and from 7 to 70 μs for SiGe-2.

Figure 4 shows Arrhenius plots for the dependences of the values of τ_m for peak A on $1/T$ in all structures. It is seen that the activation energies for peak A are different in different temperature ranges. The activation energies $E_a^{\exp}$ extracted from Arrhenius plots using expression (1) are listed in Table I. Negative values of activation energy (see, e.g., Fig. 4 for SiGe-2) observed for some structures can be caused by two possible reasons. (1) The power of T in the pre-exponential factor in expression (1) is uncertain. Really, one used different powers of T analyzing parameters of QWs examined by DLTS by means of the expression like (1): $T^{1/2}$ (Refs. 6 and 7) T^1 (Ref. 8), T^2 (Refs. 9 and 10), and even T^0 (Ref. 11). Note that there is very pronounced dependence of extracted energies on this approximation at relatively low ($E_a<0.1$ eV) activation energies. (2) A probability of level recharging can decrease with increasing temperature due to peculiarities of tunneling process taking part in QW recharging.

To determine the origin of activation energies extracted from the Q-DLTS spectra, the simulation of confined level spectra in strained *p*-SiGe QW was performed. The method used was an analog to that in Ref. 12 (see also Ref. 13 and

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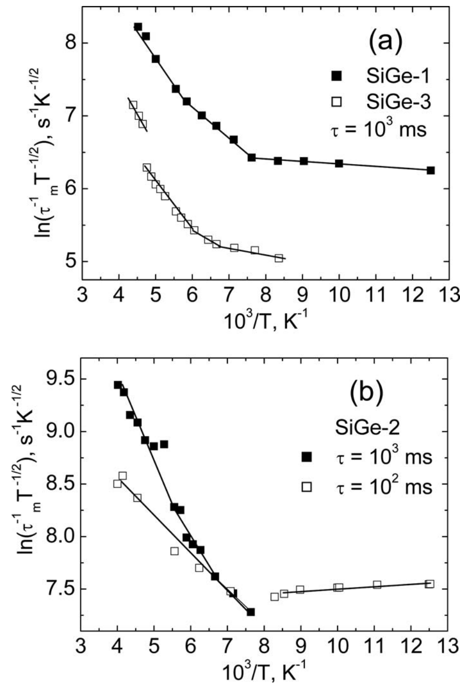

FIG. 4. Arrhenius plots for structures SiGe-1, SiGe-3 (a), and SiGe-2 (b) in the temperature range of 80–300 K. τ is duration of filling pulse. Energies extracted from these plots are given in Table I.

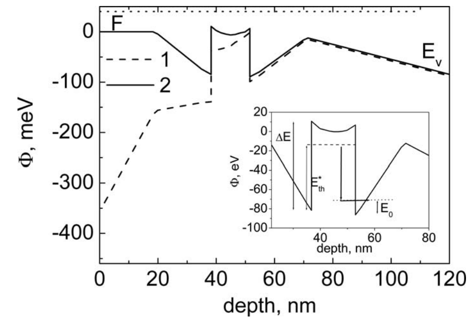

FIG. 5. Calculated band diagrams as described in the text for structure SiGe-2 with passivated and nonpassivated surface. The inset shows the scheme of thermally stimulated tunneling from one of confined levels. The energy notations are given in Table I.

references within), but with taking into account the spin-orbit interaction by using a 6×6 Luttinger Hamiltonian (instead of the 4×4 Hamiltonian used in Ref. 12). The boundary conditions applied were the continuity of wave functions and fluxes at the QW boundaries. The calculations showed that the spin-orbit interaction gives considerable contribution to the energy of excited states with index $n>2$. The calculated band diagrams for structure SiGe-2 with the passivated and nonpassivated surfaces are given in Fig. 5. The simulated confined level energies E_{th} (counted from the top of nonquantized heavy-hole subband) are given in Table I. The values $E_{th}{}^*$ also listed in Table I are the energies of the same levels counted from the valence band edge in Si barrier, which should correspond to the activation energies.

It is seen from Table I that the experimental activation energies $E_a{}^{exp}$ do not agree with the calculated energies $E_{th}{}^*$ of size quantization in QW. However, 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 (Fig. 5), which form triangle barriers. In this case, the activation energy $E_a{}^{exp}$ should be the difference between the confined state energy $E_{th}{}^*$ and some value E_0 corresponding to the optimal energy of thermostimulated tunneling. The values of E_0 found as $E_0=E_{th}{}^*-E_a{}^{exp}$ are also given in Table I.

The optimal tunneling energy for a triangle barrier can be found as energy of maximum of the total index of exponential functions of thermal emission rate and tunneling probability in dependence on carrier energy E,

TABLE I. Parameters of QW. ΔE is the valence band offset, E_{th} is the calculated energy of a confined level in the QW counted from the top of nonquantized heavy-hole subband (from the bottom of well), $E_{th}{}^*=\Delta E-E_{th}$, $E_a{}^{exp}$ is the activation energy extracted from Q-DLTS measurements in the corresponding temperature range ΔT, and $E_0=E_{th}{}^*-E_a{}^{exp}$ is the energy of optimal tunneling.

Sample, Ge content, ΔE (meV)	E_{th} (meV)	$E_{th}{}^*$ (meV)	$E_a{}^{exp}$ (meV)	ΔT (K)	E_0 (meV)
SiGe-1	37	29	3	$80<T<130$	26
7% Ge	24	42	36	$130<T<180$	13–6
66	17	49			
	4	62	61	$180<T<250$	1
SiGe-2	41	51	−8	$80<T<120$	58
10% Ge	30	62	29	$120<T<140$	33
92	18	74	41	$140<T<250$	33
	5	87	54	$170<T<250$	33
SiGe-3	77	59	11	$100<T<140$	48
15% Ge	55	81	28	$140<T<165$	53
136	44	92	57	$165<T<200$	40–35
	39	97			
	20	116	83	$200<T<220$	33
	5	131	93	$220<T<250$	38

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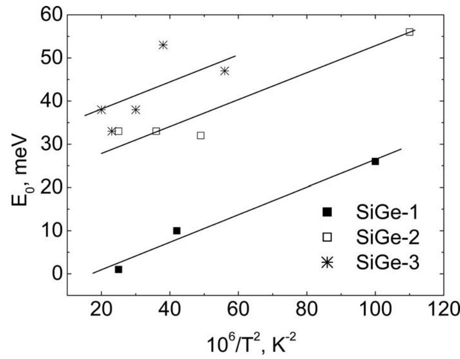

FIG. 6. Dependence of the optimal tunneling energy found as $E_0 = E_{th}^* - E_a^{exp}$ on $1/T^2$ for all investigated structures.

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

where m is the carrier effective mass, e is the elementary charge, k is the Boltzmann constant, and F is the electric field strength at the triangle barrier. The emission rate at thermally stimulated tunneling is then given by the expression [see, e.g., (10.21) in Ref. 13]

$$p(F) = \exp\left[-\frac{E_{th}^*}{kT} + \frac{1}{6mkT}\left(\frac{eF\hbar}{2kT}\right)^2\right] = \exp\left[-\frac{1}{kT}(E_{th}^* - E_{0th})\right], \quad (3)$$

$E_{0th} = (1/6m)(eF\hbar/2kT)^2$ is the lowering of potential barrier due to tunneling, which should be compared to the experimental value of E_0. Figure 6 shows the dependence of E_0 on T^{-2} for Si/SiGe/Si structures with different Ge contents. The numerical estimation of effective mass, which is needed to fit the slopes of these dependences by expression (3), gives $m = 0.45m_0$ (m_0 is the free electron mass) at the electric field strength $F = 1.8 \times 10^5$ V/cm extracted from simulation for applied voltage used for the Q-DLTS measurements. This value of m is consistent with the experimental m values obtained for SiGe/Si structures.[14,15] As seen in Fig. 6, the dependences $E_0(T^{-2})$ are shifted to higher energies for the structures with higher Ge content. It can be connected with a change in confined energy values caused by a distortion of QW potential profile in the external electric field.

IV. CONCLUSIONS

The surface passivation of Si/SiGe/Si structures with organic monolayers of 1-octadecene was found to remove the surface defect charge, change the potential distribution across the structure, and lead to a higher population of holes in SiGe QWs. The surface passivation allowed us to observe the excitation of confined levels in Q-DLTS measurements for SiGe QWs with different Ge contents. The carrier emission was observed not only from the first but also from the second and higher energy levels of light and heavy holes. The different hole levels were observed as the different slopes of the Arrhenius plot for a particular Q-DLTS peak in different temperature ranges. Comparison of these activation energies with the calculated confined energies leads to the conclusion about the decisive role of thermostimulated tunneling in carrier emission from SiGe QW.

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