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Acceptor states in boron doped SiGe quantum wells

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Abstract. The temperature dependences of lateral conductivity and hole mobility in SiGe quantum well structures selectively doped with boron are presented. The boron A^+ centers are found to exist and determine the low-temperature conductivity. The activation energy of conductivity at higher temperatures is shown to be determined by the energy distance between strain-split boron A^0 levels. The model of two-stage excitation of free holes including the thermal activation of holes from the ground to split-off state and next tunneling into the valence band is proposed. The binding energy of A^+ centers and the energy splitting of boron ground states by strain are found.

Selectively doped SiGe quantum well structures (QWs) are of great interest for study of acceptor states which are degenerate in bulk material and should be split in two-dimensional (2D) systems due to space quantization and/or strain. The energy positions of ground and excited states of an acceptor can be controlled in a wide range by alloy composition, QW width, doping level and space position of an acceptor center. So-called A^+ states (acceptors binding an additional hole) [1,2] are of specific interest as they should exist in SiGe QWs in thermal equilibrium in contrast to bulk material where they can appear only due to excitation, e.g., by light. Similar D^--states of donors have been investigated in GaAS/GaAlAs structures [3,4].

The *p*-type Si/SiGe/Si QWs MBE-grown pseudomorphically on the n-type Si substrate and selectively doped with boron were used for conductivity and magnetoconductivity measurements at the temperatures of 4 up to 300 K. The SiGe layer of 20 nm thickness was sandwiched between undoped Si buffer (130 nm wide) and cap (60 nm) layers. The SiGe QW was uniformly doped with boron; the B concentration was of 3×10^{17} cm^{-3}. The content of Ge, x, in SiGe alloy was 0.1 and 0.15, respectively. Two boron δ-layers with B concentration of 2×10^{11} cm^{-2} positioned within the buffer and cap layers on the distance of 30 nm from each QW interface were used to obtain A^+ centers inside the QW. The buffer *delta*-layer should also supply holes to form the $p-n$ junction between the p-layers and the n-substrate. The contacts were deposited on the p-type side of structures so that the p-n junction prevented from a current along the substrate.

Figure 1 shows, in log-$1/T$ scale, the temperature dependence of conductivity, σ, along the SiGe layer for the samples with 0.1 and 0.15 Ge content, x. One can see two activation-law regions in the curves. The low-temperature activation energy is

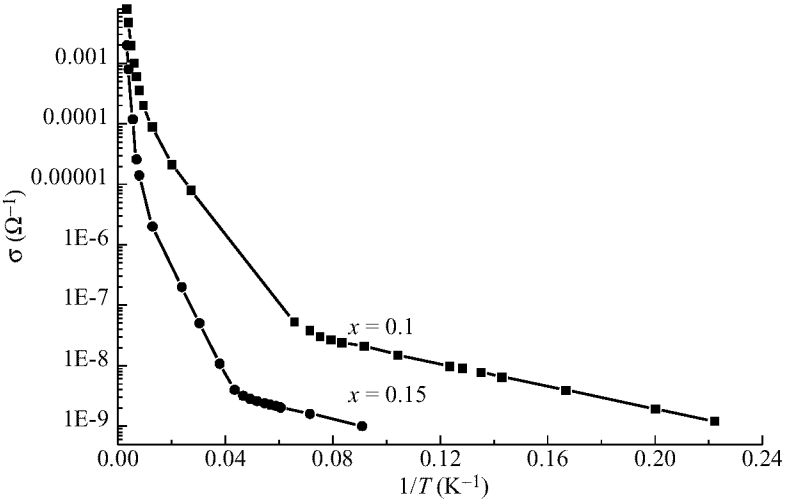

Fig 1. Temperature dependence of conductivity.

approximately 2 meV and practically coincides for the samples with different Ge content. The activation energy at higher temperatures ($T \geq 20$ K) is of 12 ± 1 meV for $x = 0.1$ and 18 ± 1 meV for $x = 0.15$. The hole mobility, μ, determined from the measurements of transverse magnetoconductivity had the maximum value of 20000 cm^2/Vs at 28 K.

There are two possible explanations for $\sigma(T)$ dependence at low temperatures. First, the activation energy (≈ 2 meV) can be due to the thermally activated hopping conductivity. In dependence on the Fermi level (ε_F) position, the hopping can be over neutral (A^0) boron states if $\varepsilon_F \approx \varepsilon_0$, ε_0 is the A^0 binding energy, or positively charged A^+ states if $\varepsilon_F \approx \varepsilon^+$, it is A^+-centers binding energy. The main argument against the hopping is the low conductivity observed. Really, at the given doping level in QW, 3×10^{17} cm^{-3}, the mean distance between impurities (≈ 8 nm) is of the order of the effective Bohr radius of impurity, which can be estimated by the expression $a_B \approx \hbar/\sqrt{2m\varepsilon_B}$. Using linear interpolation of GeSi parameters between Si and Ge, we get $a_B \approx 2.5$ nm for A^0 and ≈ 10 nm for A^+ states [5]. Because of strong overlapping impurity states, the specific (on square) conductivity value can not be less than 10^{-3} to 10^{-4} Ω^{-1} (see, f.i., [6] for references). It is several orders of magnitude more than the experimental values.

The second possible origin of 2 meV activation energy can be the thermal hole emission from A^+ states. The calculation of the A^+ binding energy [7] gives just $\varepsilon^+ \approx 2$ meV, being weakly dependent on Ge content in SiGe alloy. The calculated temperature dependences of free hole concentration are shown in Fig. 2. The parameters for the best fit of calculate and experimental curves were found to be $\varepsilon_0 = 24$ meV and 36 meV for $x = 0.1$ and $x = 0.15$, respectively, $\varepsilon^+ = 2$ meV and $N^+ = 10^9$ cm^{-2} for both structures (N^+—is the A^+-center concentration in the QW). Thus, the low-temperature activation energy is the binding energy of the boron A^+ centers in QW. However, the extra hole concentration supplied into QW turns out to be two orders less than the doping level of δ-layers. The only reason for this seems to be Si surface states which can accumulate almost all holes from the δ-layers.

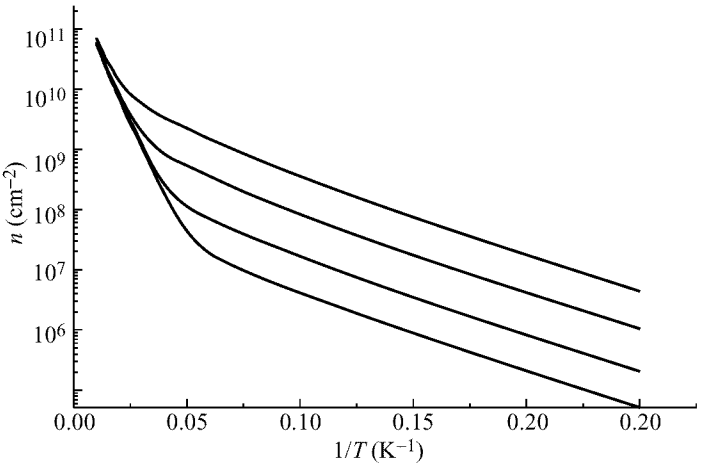

Fig 2. Calculated temperature dependence of hole concentration in QW at various δ-layer doping level.

The origin of activation energy at higher temperatures is not so obvious. It should be one half of boron-A^0 binding energy because the Fermi level lies between the valence band edge and the B^0 ground state as it is filled. So, the observed high-temperature activation energies, 12 and 18 meV, should correspond to 24 and 36 meV B^0 binding energies. These values are, however, quite surprising. Indeed, the binding energy of shallow impurity should decrease with increasing both Ge content and strain, it is quite the contrary to the experiment. Moreover, the value of $\varepsilon_0 = 24$ meV seems not to be real for $x = 0.1$. The only energy which could agree with the above values of ε_0 is the energy difference between acceptor levels split by strain. Indeed, the splitting energy of the ground acceptor state found by means of linear interpolation between Si and Ge is $\approx$ 15 and 25 meV for $x = 0.1$ and $x = 0.15$, respectively. This is close to the experimental activation energies. (Note that the estimation of the energies by interpolation is very approximate.) The splitting energy can be as the activation one only if holes can pass from the split-off state into the valence band without activation, that is by tunneling. It is impossible in the scheme of flat bands. On the other hand, we have seen from the experiment that almost all holes from the δ-layers accumulate in the surface states making the surface charged. So, the potential across the structure should appear inclining the valence bands. The scheme of potential distribution for this case is shown in Fig. 3. One can see from this scheme that the conductivity in this case can be controlled by two-stage process: first, the thermal activation of holes from the ground to split-off state takes place and then hole tunneling into free hole band creates the conductivity. To estimate the possible potential drop across the structure, let's remember an empirical law that for most homeopolar semiconductors the Fermi energy is fixed on the surface near 1/3 of the energy gap from the valence band. It is $\approx$ 0.4 eV for Si. The QW width is 5 times less than the structure width. So, the potential drop on the QW is of $\approx$ 80 meV. Of course, this estimation is too rough but it shows that the proposed model can be real. Thus, the arguments for the model are (i) the increasing activation energy of conductivity with Ge content, (ii) small additional

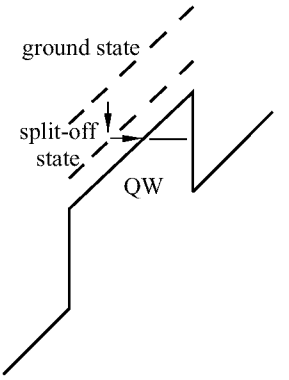

Fig 3. Scheme of conductivity activation by tunneling.

hole concentration supplied from δ-layers into the QW, and (iii) charging the surface and arising the potential drop across the QW, as a consequence.

The experimental data presented give evidence for existence of A^+ centers in B doped SiGe QW structures in thermal equilibrium. The thermal emission of holes from these centers determines the conductivity along the QW at low temperatures. At higher temperatures, the conductivity is shown to be due to thermal activation of holes from the ground to strain-split B states following by hole tunneling into the QW valence band. The tunneling is possible due to a potential drop across the QW which arise due to hole capture at surface states of the Si cap layer making the surface charged. Note that in structures with doping profile and level investigated, it is possible to find the energy splitting of acceptor levels by strain from temperature dependence of conductivity.

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