Localized-state band induced by B δ-doping in $Si/Si_{1-x}Ge_x/Si$ quantum wells

K. Schmalz
Institute for Semiconductor Physics, Walter-Korsing-Strasse 2, 15230 Frankfurt (Oder), Germany

I. N. Yassievich
Ioffe Physico-Technical Institute, 26 Polytechnicheskaya, 194021 St. Petersburg, Russia

K. L. Wang and S. G. Thomas
UCLA Electric Engineering Department, University of California, 66-147 Engineering IV, 405 Hilgard Avenue, Los Angeles, California 90095-1594

(Received 16 September 1996; revised manuscript received 3 June 1997)

The density of states of the two-dimensional hole band in B δ-doped $Si/Si_{1-x}Ge_x/Si$ quantum wells was obtained using space-charge spectroscopy. $Si/Si_{0.75}Ge_{0.25}/Si$ structures studied have a $(2-5)\times10^{11}$ cm^{-2} concentration of B δ doping in the middle of the quantum well. We have observed the effect of localization for small concentrations of confined holes. The activation energy for the hole emission rate increases as the concentration of confined holes decreases. This allows one to estimate the density of states for the tail of the two-dimensional acceptor band. [S0163-1829(98)01211-9]

I. INTRODUCTION

Boron-doped $Si_{1-x}Ge_x$ layers in silicon are candidates for use in high-speed or other devices integrated with silicon-based circuits.[1] Various infrared detectors[2] have been demonstrated using these layers. They may also be potentially used for far-infrared (terahertz) emitters and lasers.[3]

However, little information is available on the density of states and mobility of confined holes in these layers. For example, it is not clear how the energy position of acceptor states changes with the $Si_{1-x}Ge_x$ layer width, the Ge concentration, or the location of the acceptors in $Si/Si_{1-x}Ge_x/Si$ layers. It is also not known how extended states are formed as the boron concentration increases. Strongly correlated two-dimensional carrier systems are now under intensive study, including the question of an metal-insulator transition in such systems.[4–6]

Here, we present an investigation of boron δ-doped quantum $Si_{1-x}Ge_x$ layers by space charge spectroscopy, and demonstrate the possibility to determine the density of states of a two-dimensional impurity band.

Deep-level transient spectroscopy (DLTS) is a standard technique for measuring the activation energy of carrier emission from deep levels. In applying DLTS to studying carrier emission from quantum-well (QW) structures, the lateral diffusion of confined carriers causes a problem that the carriers are swept from the QW region laterally beneath the Schottky contact before hole emission across the barrier can occur. Direct hole emission from $Si/Si_{1-x}Ge_x/Si$ QW structures was observed for narrow QW's (2–3 nm) with high Ge concentrations ($x=0.3-0.5$).[7] It was easier to observe direct hole emission in this case as the alloy and interface interface scattering reduces the hole mobility. A low hole mobility is also expected for boron δ-doped quantum $Si_{1-x}Ge_x$ layers. Thus the hole emission can be conveniently studied by DLTS. In the case of DLTS the confined hole concentration can be changed in the QW layer by applying a reverse bias. The dependence of the activation energy of the hole emission rate on the concentration of confined holes gives the possibility to obtain information on the density of states of the two-dimensional boron impurity band.

In this study, we used $Si/Si_{0.75}Ge_{0.25}/Si$ QW structures. The concentration of boron δ doping, N_B, in the middle of the $Si_{0.75}Ge_{0.25}$ layer is $N_B=(2-5)\times10^{11}$ cm^{-2}. Note that $N_B<N_c$ where $N_c\approx1.5\times10^{12}$ cm^{-2} is the critical concentration of B in Si for the Mott metal-insulator transition in a disorder two-dimensional layer. For estimating N_c the condition $N_c^{1/2}a^0\approx0.37$ is used,[8,9] where a^0 is the effective Bohr radius given by the relation $a^0=(2m_1E_A)^{1/2}/\hbar$ equal to 2.3 nm, with the experimental value of the binding energy $E_A=45$ meV, and the light hole mass $m_1=0.16\,m_0$ calculated in spherical approximation. The critical concentration N_c should be smaller in the case of $Si_{0.8}Ge_{0.2}$. A calculation with a linear interpolation of the parameters for SiGe gives $E_A=37$ meV, $m_1=0.14m_0$, $a^0=2.7$ nm, and corresponding $N_c=1.9\times10^{12}$ cm^{-2}. Thus, for our boron δ-doping condition localization is expected for the first impurity band formed by boron.

In the equilibrium condition, the concentration of holes n_w confined in the QW should exceed N_B; holes are supplied from the barrier layers. At low temperatures these additional holes should occupy the second Hubbard subband, which results from the A^+ states (charged acceptor states). The small binding energy of A^+ states (for boron in bulk Si about 2 meV) results in a lower critical concentration for the metal-insulator transition. In this case we obtain an effective radius of about 12 nm for separated A^+ states and correspondingly, a critical concentration $N_c=1\times10^{11}$ cm^{-2}, which is smaller than our boron δ-doping concentration. Thus the condition of the existence of metallic states should be realizable here. By applying a reverse bias to our $Si/Si_{1-x}Ge_x/Si$ QW structure, the confined hole concentration can be redirected in a wide range and a metal-insulator transition can be obtained.

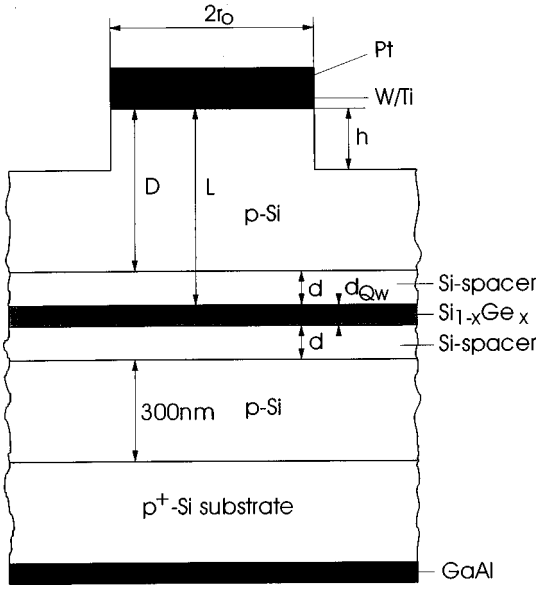

FIG. 1. Schematic picture of the mesa WTi Schottky diode used.

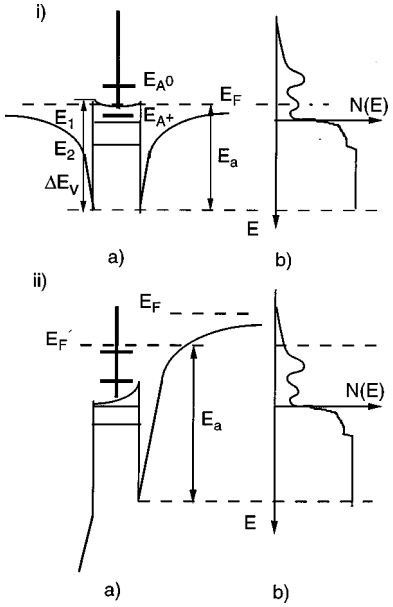

FIG. 2. Schematic view of (a) valence-band profile and (b) distribution of the density of states $N(E)$: (i) equilibrium conditions and (ii) nonequilibrium conditions. The energy levels of an isolated neutral acceptor E_{A^0} and of a charged acceptor E_{A^+} are shown, as well as Fermi level E_F in equilibrium condition, quasi-Fermi-level E_F' in nonequilibrium condition, and the activation energy E_a.

No gap between the extended and localized states is evident in these boron δ-doped quantum $Si_{1-x}Ge_x$ layers. However, we observed a ''freeze out'' of the holes to deeper states; a typical behavior of a strongly correlated two-dimensional carrier system, where the amplitude of random potential fluctuations (disorder) decreases with increasing concentration of confined holes. The dependence of the hole emission rate on the concentration n_w of confined holes gives information on the density of states for the case $n_w < N_B$.

II. EXPERIMENT

A. Sample preparation

The p-type $Si/Si_{1-x}Ge_x/Si$ structures used in the present work were grown pseudomorphically at 530 °C in a molecular-beam epitaxy (MBE) system. The epilayers were deposited onto (100) p^+-Si substrates, B doped, with a resistivity of 0.01–0.02 Ω cm. First, a 300-nm-thick buffer, B-doped with about 10^{17} cm^{-3}, was grown. For the structures the $Si_{0.75}Ge_{0.25}$ layers were sandwiched between 30 nm undoped Si spacers. The following structures were investigated: (1) SiGe layer thickness $d_{SiGe}=5$ nm, undoped; (2) boron δ doping in the middle of the SiGe layer with a surface concentration of 2×10^{11} cm^{-2}, $d_{SiGe}=5$ nm; (3) boron δ doping in the middle of the SiGe layer with 5×10^{11} cm^{-2}, $d_{SiGe}=4$ nm. The thickness d_{SiGe} was determined by transmission electron microscopy (TEM). Finally, a 300-nm-thick B-doped Si cap layer with a dopant concentration of about 10^{17} cm^{-3} was deposited (Fig. 1).

Schottky diodes were prepared by W/Ti deposition. The effective area of the Schottky contact was $A=1.3\times10^{-2}$ cm^2. For the CV and DLTS investigations, we also used structures for which the thickness of the cap layer was reduced by chemical etching to obtain an optimal thickness for these investigations. For DLTS measurements, we used a mesa Schottky diode geometry (Fig. 1), such that the $Si_{1-x}Ge_x$ layer did not penetrate the mesa, but formed a buried layer. The DLTS measurements were performed with the DLTS spectrometer DLS-82 of SEMILAB, Hungary, and CV and admittance investigations were carried out using a HP 4192 A low-frequency impedance analyzer.

B. Admittance spectroscopy and capacitance voltage measurements

The $Si/Si_{1-x}Ge_x/Si$ structures having a 300-nm-thick cap layer and an acceptor concentration N_A of about 10^{17} cm^{-3}, the SiGe layer is outside the Schottky barrier depletion width at zero reverse bias ($U_R=0$). The activation energy E_a of conductance across the QW can be obtained using admittance spectroscopy.[10] From the equivalent circuit of the space-charge region of the Schottky diode and the QW, one obtains C_p and G_p (capacitance C and conductance G measured in a parallel equivalent circuit) as function of C_1, C_2, and G, where C_1 is the capacitance of the space-charge region of the Schottky diode, C_2 the capacitance of the QW, and G the conductance across the QW.[10] A maximum in $G_p(T)$ appears at $G^*=2\pi f(C_1+C_2)$.

The temperature dependence of the conductance, G, across the QW is given by $G(T\sim T^{1/2}\exp(-E_a/k_BT)$. Hence, the activation energy E_a is estimated from the Arrhenius plot of the measurement frequency f versus $1/T$, at which the conductance peak occurs.

If the SiGe layer is undoped (sample 1), the activation energy $E_a=69$ meV is well approximated by $E_a\approx\Delta E_v - E_1$, where ΔE_v is the valence-band offset and E_1 is the confinement energy of the first level of the heavy hole in the QW.[10] Figure 2 shows the important potentials and energies for two-dimensional system under investigation. The Arrhenius plot of the measurement frequency f gives an activation energy of $E_a=75$ meV for the structure with a B δ concentration of 2×10^{11} cm^{-2} (sample 2); for the structure with a B δ concentration of 5×10^{11} cm^{-2} (sample 3), a somewhat

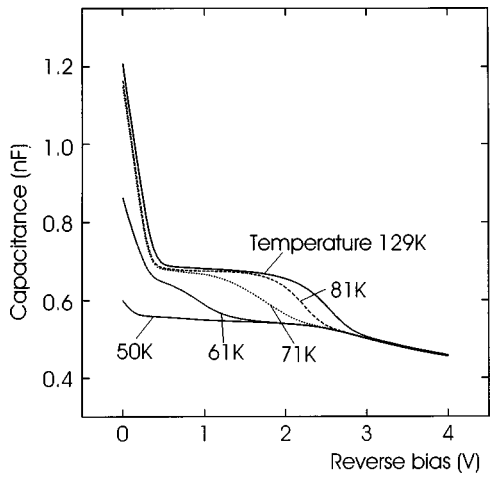

FIG. 3. Dependence of the capacitance C on reverse bias U_R for 1 MHz measurements at different temperatures (sample 2; thickness of the cap layer 150 nm, effective area of the Schottky contact $A = 1.2\times10^{-2}$ cm^2): (a) 50 K, (b) 61 K, (c) 71 K, (d) 81 K, (e) 129 K.

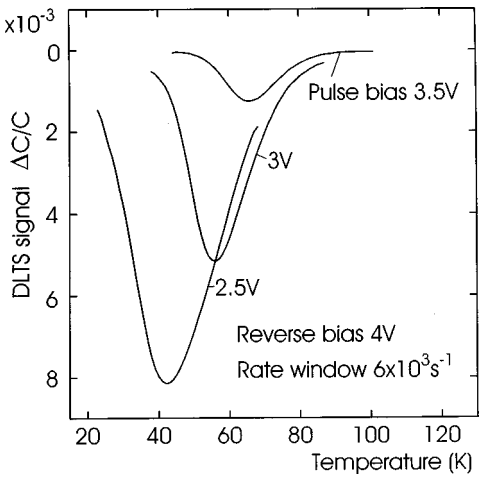

FIG. 4. DLTS spectrum (sample 2; thickness of the cap layer 200 nm) at the reverse bias $U_R = 4.0$ V and pulse frequency $f = 2500\ \mathrm{s}^{-1}$ (corresponding to emission rate window $e_0 = 5580\ \mathrm{s}^{-1}$) for different pulse biases U_1: (a) 2.5 V, (b) 3.0 V, and (c) 3.5 V. The pulse duration was $t_p = 5\ \mu$s.

smaller activation energy of $E_a = 51$ meV was obtained. This appears reasonable for the smaller SiGe thickness of 4 nm for sample 3 compared to 5 nm for sample 2 as previous calculations show.[10]

The dependence of the capacitance C on the reverse bias U_R, shown in Fig. 3 for sample 2 (with a B δ concentration 2×10^{11} cm^{-2}) reveals a plateau of nearly constant capacitance C^*. The plateau between the first and second biases U_{R1} and U_{R2} is related to the hole concentration in the QW by $n_w = C^*(U_{R2}-U_{R1})/Ae$, where A is the diode area and e is the elementary electron charge.[10] We have estimated the maximum hole concentration n_w to be about 10^{11} cm^{-2} for the structure with undoped SiGe, and correspondingly for the δ-doped cases $n_w = 3\times10^{11}$ cm^{-2} for 2×10^{11} cm^{-2} B, and $n_w = 5.5\times10^{11}$ cm^{-2} for 5×10^{11} cm^{-2} B. In the case of the B-doped SiGe layer, the concentration n_w measured is equal to the total hole concentration in the QW layer, i.e., the concentration of holes supplied from the barriers plus the B δ-doped layers. Note that the relation $N_B < n_w < 2N_B$ is fulfilled for the confined hole concentration n_w, i.e., the Fermi level E_F should lie in the second (Hubbard) subband at low temperatures (Fig. 2). The close values of activation energies measured for the B δ doped and the undoped QW's show that in the case of our B δ doping the larger part of holes lie in the two-dimensional band of free holes at the measurement temperatures (in the range 60–80 K), i.e., below the confinement level E_1 (Fig. 2).

For CV measurement, only holes with an emission rate e_T larger than the angular frequency $\omega = 2\pi f$ contributes to the plateau in capacitance. Figure 3 shows the $C = C(U_R)$ dependencies for different temperatures measured at the measurement frequency f. The width of the capacitance plateau decreases with decreasing temperature indicating that an increasing part of the hole concentration n_w is characterized by a lower emission rate $e_T < \omega$. Such behavior suggests a wide range of activation energies for hole emission. This indicates a ''freeze out'' of the holes to deeper states. The CV characteristics, measured at a given temperature for different frequencies, show a similar behavior. The ''frozen-out'' holes are released only at a larger reverse bias, leading to a second plateau in the CV curve.

C. DLTS measurements

We obtained the minimum reverse bias U_R^*, at which the QW becomes depleted, from the $C = C(U_R)$ dependencies measured at various temperatures. For this condition, we performed DLTS measurements. A strong DLTS signal related to hole emission from the QW was observed for the B δ-doped Si/Si$_{1-x}$Ge$_x$/Si structures (Fig. 4), but not for the structure with undoped SiGe layer. This difference is probably due to the different lateral hole diffusion in the SiGe layer for the two cases.[7] The hole diffusivity in the SiGe layer for the doped sample is lower than for the undoped SiGe. The DLTS peak temperature and the peak shape depend considerably on the pulse bias U_1, e.g., for larger pulse amplitude $(U_R^* - U_1)$ a broadening of the DLTS peak at the lower-temperature side occurs, indicating a ''tail'' of localized states in the QW (Fig. 4).

The maximum emitted hole concentration n_w^* was estimated from the DLTS signal $(\Delta C/C)$ from the relation $n_w^* = (\Delta C/C)(2N_A W^2/L)$, with $\Delta C/C$ at the measurement frequency $f = 2500\ \mathrm{s}^{-1}$. Here, N_A is the acceptor concentration in the buffer layer, L is the thickness of the Si layer between the Schottky contact and SiGe layer, and W is the width of the depletion region. We have calculated the activation energy E_a of hole emission from the Arrhenius plot of the hole emission rate e_T. Figure 5 shows the Arrhenius plots of the hole emission rate e_T for a QW with various nonequilibrium hole concentrations n_w^*, which were realized by various pulse bias amplitudes U_1. The activation energy E_a, calculated from the DLTS measurements for larger hole concentration n_w^*, is in good agreement with that obtained by admittance spectroscopy. For a smaller hole concentration in the QW, the activation energy increases significantly, as shown in Fig. 6.

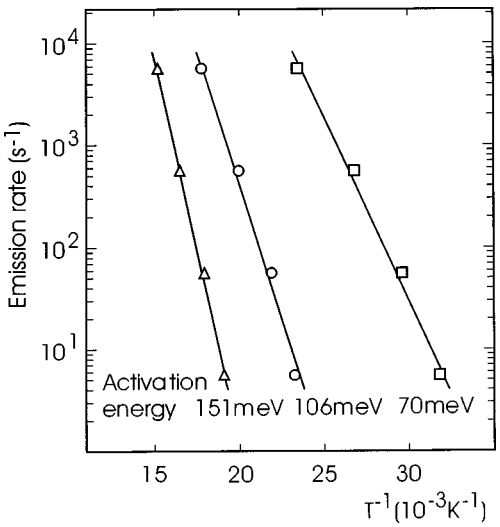

FIG. 5. Arrhenius plot of the hole emission rate e_T (sample 2; thickness of the cap layer 200 nm) at the reverse bias $U_R = 4.0$ V. The pulse bias U_1 is varied: (□) 2.5 V, (○) 3.0 V, and (△) 3.5 V, corresponding to the following nonequilibrium hole concentration n_w^* (obtained from the DLTS peak $\Delta C/C$ at $f = 2500\ \mathrm{s}^{-1}$): (□) 3×10^{10} cm^{-2}, (○) 2×10^{10} cm^{-2}, and (△) 5×10^{9} cm^{-2}.

III. DISCUSSION

Holes confined in a QW with a high δ-doping concentration give rise to a two-dimensional system with random potential fluctuations.[4,5] In equilibrium, as realized for admittance spectroscopy, the concentration of confined holes n_w is larger than the doping concentration N_B of boron. In this case, one can assume that some of the holes are located in the upper subband induced by B δ doping (Fig. 2). Therefore, we expect that a two-dimensional low-mobility metal is realized.[6] But for DLTS, when applying a large reverse bias to the structure, the concentration of confined holes n_w^* is smaller than N_B. In this case, we have a strongly localized confined hole system, where the lateral conductivity σ in the QW is expected to decrease with temperature according to an activation law:

$$\sigma \sim \exp(-\varepsilon_a / k_B T), \tag{1}$$

where ε_a is the energy separation between the mobility edge ε_c and the ''quasi-Fermi-level'' E_F' which is a function of the hole concentration n_w^*. It is reasonable to assume that the activation energy ε_a for conductivity should strongly increase as the hole concentration is reduced.[5,11,12] (Note, we can introduce a ''quasi-Fermi-level'' for the characterization of nonequilibrium holes in a QW, because the space and energy redistributions among confined holes occur faster than the hole emission process during the DLTS measurement.)

The lateral hole diffusivity should also follow the activation law given by Eq. (1). This allows us to observe a DLTS signal for small confined hole concentrations of ($\leqslant 3\times10^{10}$ cm^{-2}). On the other hand, for larger hole concentrations, the lateral hole diffusivity becomes large enough to reduce considerably the hole concentration beneath the Schottky contact during the measurement time of DLTS $1/f$, and thus a DLTS signal can not be observed.

The activation energy E_a of hole emission is determined by the difference between the potential barrier U at the QW and the Fermi level E_F (Fig. 2). The admittance spectroscopy data give an E_a between 75 meV (at 2×10^{11} cm^{-2} B) and 51 meV (at 5×10^{11} cm^{-2} B) for an equilibrium hole concentration n_w, when n_w is larger than the B δ concentration N_B. The observed ''freeze out'' of holes by CV measurements at lower temperatures (Fig. 3) suggests the existence of an impurity band. However, we have no evidence for a gap between the extended and localized states.

The observed strong DLTS signal (Fig. 4) indicates a strong localization of confined holes when $n_w < N_B$. There is a strong increase in the activation energy E_a with decreasing hole concentration (Fig. 6). Using this dependence, we have calculated the density of states $N(E)$ related to the activation energy. This density of states $N(E)$ corresponds to the thermodynamic density of states introduced for the characterization of two-dimensional electron systems with disorder by the relation $N(E) = dn_w/dE_F$.[11–13] $N(E)$ was obtained from the experimental results by the relation $N(E) = n_w^*/(0.48 k_B T)$ in a way similar to that previously reported for the DLTS characterization of the interface state distribution.[14] The factor 0.48 is due to the signal averaging by lock-in technique used for our DLTS spectrometer.[14] The energy E is taken as $E = E_a^{\mathrm{adm}} - E_a^{\mathrm{DLTS}}$, where E_a^{adm} and E_a^{DLTS} are the activation energies measured by admittance spectroscopy and DLTS, respectively. The dependence of the density of states $N(E)$ on the energy is given in Fig. 7. The value $E = 0$ corresponds to the Fermi level when the two-dimensional band of free holes is in equilibrium and is close to the energy position E_1 (Fig. 2).

The observed dependence $N(E)$ is considerably weaker than $N(E) \sim \exp(-E/\Delta V)$ with $\Delta V = 0.5\, e^2 N_B / 4\pi\varepsilon_0\varepsilon_r (n_w)^{1/2}$ ($\varepsilon_0\varepsilon_r$ is the dielectric constant). Such a dependence would be expected for a random distribution of boron dopants and a carrier screening within the framework of the classical model for $n_w \ll N_B$ and for n_w larger than the

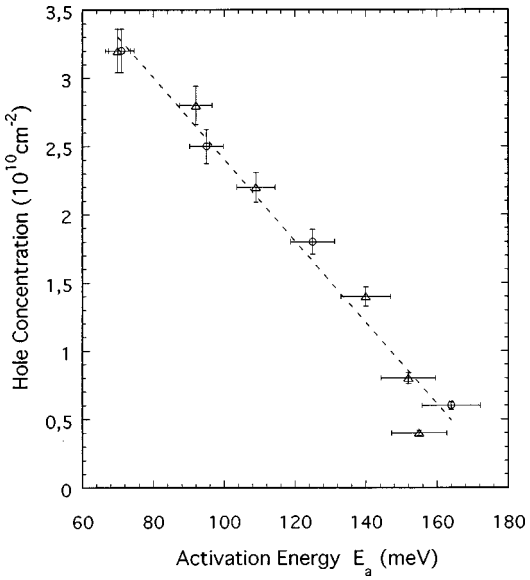

FIG. 6. Dependence of the hole concentration n_w, emitted with activation energy E_a, on the activation energy E_a: sample 2 (△), and sample 3 (○).

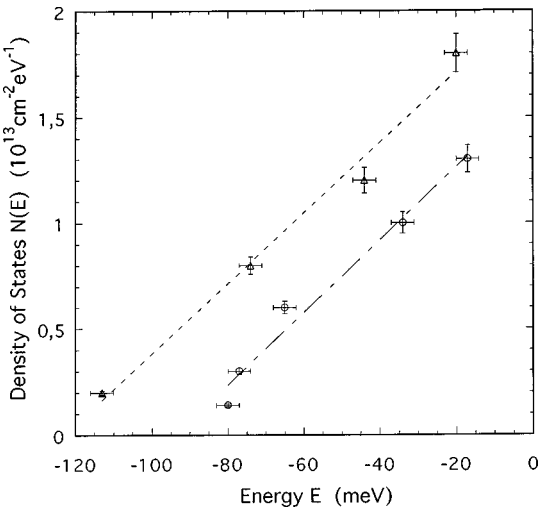

FIG. 7. Dependence of the thermodynamic density of states $N(E)$ on the energy E, where $E=0$ corresponds to the edge of the two-dimensional band of free holes: sample 2 (dash-dot line), and sample 3 (dashed line).

residual concentration of compensating impurities.[6] Note, that in our case the effective Bohr radius a^0 is practically equal to d_{SiGe}, and the B δ-doped layer is in the middle of the QW. Previously, problems of random potential and screening effect by confined carriers were investigated for the case of a δ-doped layer separated by a spacer from the QW layer.[11,12] Applying these results to our structures, we have estimated the average amplitude of the random potential in the QW plane in the absence of confined holes by using the following relation:

$$(\langle \Delta V^2 \rangle)^{1/2} = (2\pi)^{1/2}(e^2/4\pi\varepsilon_0\varepsilon_r)(N_B)^{1/2}[\ln(R_A/d_{\mathrm{SiGe}}]^{1/2}. \quad (2)$$

Here we have used $d_{\mathrm{SiGe}}/2 \approx a^0$ instead of the spacer width, and the radius (R_A) of the Schottky contact as the characteristic length along the QW plane. As a result, we have obtained $(\langle \Delta V^2 \rangle)^{1/2} = 42$ meV for $N_B = 2\times 10^{11}$ cm^{-2}. This estimation is in reasonable agreement with the observed increase of the activation energy. The screening effect should strongly reduce the random potential with increasing confined hole concentration at a relatively low hole concentration in the regime of nonlinear screening.[11,12] In this regime, the hole density is very nonhomogeneous in the QW plane for the scale of the order R_A. The characteristic amplitude of the random potential, which separates local regions occupied by holes, is of the order $(e^2/4\pi\varepsilon_0\varepsilon_r)(N_B)^{1/2}$. Thus, an activation law (1) for conductivity (isolation regime) takes place here, and conditions for DLTS study are fulfilled.

IV. SUMMARY

In summary, we have studied acceptor states induced by boron δ doping in SiGe QW layers using space charge spectroscopy. We have observed a strong dependence of the activation energy for hole emission from the QW on the concentration of confined holes. The observed transport properties of the confined holes for hole concentrations smaller than the B δ doping concentration are typical for a strongly localized two-dimensional disordered hole system. Finally, we have determined the density of states near the tail of the two-dimensional band, when the hole concentration in the SiGe QW layer is smaller than the concentration of the boron δ doping.

ACKNOWLEDGMENTS

We are indebted to A. Ourmazd for a critical reading and useful comments. We acknowledge the support of the Volkswagen-Stiftung. We would like to express our gratitude to R. Winkler for technical assistance. The UCLA effort was in part supported by NSF and SRC.

[1] T. K. Carns, X. Zheng, K. L. Wang, S. L. Wu, and S. J. Wang, J. Vac. Sci. Technol. B **12**, 1203 (1994).
[2] S. K. Chun, D. S. Pan, and K. L. Wang, Phys. Rev. B **47**, 15 638 (1993).
[3] I. N. Yassievich, K. Schmalz, M. A. Obnoblyudov, and M. S. Kagan (unpublished).
[4] S. V. Kravchenko, Whitney E. Mason, G. E. Bowker, and J. E. Furneaux, Phys. Rev. B **51**, 7038 (1995).
[5] A. L. Efros and F. G. Pikus, Solid State Commun. **96**, 183 (1995).
[6] N. F. Mott, *Metal-Insulator Transitions* (Taylor & Francis, London, 1991).
[7] K. Schmalz, I. N. Yassievich, E. J. Collart, and D. J. Gravesteijn, Phys. Rev. B **54**, 16 799 (1996).
[8] B. I. Shklovskii and A. L. Efros, *Electronic Properties of Doped Semiconductors* (Springer, Heidelberg, 1984).
[9] A. G. Kyazym-zade, Fiz. Tekh. Poluprovodn. **29**, 1915 (1995) [Semiconductors **29**, 10 (1995)].
[10] K. Schmalz, I. N. Yassievich, H. Rücker, H. G. Grimmeiss, H. Frankenfeld, H. J. Osten, P. Schley, and H. P. Zeindl, Phys. Rev. B **50**, 14 287 (1994).
[11] A. L. Efros, Phys. Rev. B **45**, 11 354 (1992).
[12] A. L. Efros, F. G. Pikus, and V. G. Burnett, Phys. Rev. B **47**, 2233 (1993).
[13] T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[14] D. Vuillaume, J. C. Bourgoin, and M. Lannoo, Phys. Rev. B **34**, 1171 (1986).