

Hopping conduction and field effect in Si modulation-doped structures with embedded Ge quantum dots

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(Received 23 September 1998)

We report measurements of hopping transport in modulation-doped Si field-effect structures with a layer of Ge nanometer-scale dots embedded in proximity with the *p*-type conductive channel. It is found that the activation energy of hopping conductivity in the impurity band of the doped Si layer changes with increasing quantum dot (QD) size, passing through a minimum, due to trapping of holes by the QD's. We observed conductivity oscillations with the gate voltage which disappeared in magnetic field. The drain current modulation was attributed to hopping transport of holes through the discrete energy levels of the Ge nanocrystals. Field-effect measurements in structures which contain as many as 10^9 dots enable us to resolve as well-pronounced maxima in $G - V_g$ characteristics the single-electron charging of each dot with up to six holes. The level structure reveals up to three distinct shells which are interpreted as the *s*-like ground state, the first excited *p*-like state and the second excited *d*-like state. We are able to obtain the hole correlation (charging) energies in the ground and first excited states, the quantization energies and the localization lengths.

[S0163-1829(99)08819-0]

I. INTRODUCTION

Epitaxial growth of highly strained materials in the Stranskii-Krastanov growth mode enables *in situ* fabrication of dense arrays of nanometer-scale high-quality quantum dots (QD's) which can be considered as artificial atoms. Most of the experimental and theoretical works¹⁻¹⁰ on the structural and electronic properties of such self-assembled QD's have concentrated on the heterosystem InAs/GaAs. In particular, it has been found^{5,10} that InAs dots embedded in the vicinity of a two-dimensional electron gas in selectively doped heterojunctions give rise to a progressive reduction of the electron mobility, acting as controllable scattering centers. Typical densities of InAs QD's formed on GaAs substrates are about 10^{10} cm⁻² or less. Despite the current trends in microelectronics which require the development of methods for producing quantum dots in silicon-based structures, self-assembled Ge QD's on Si are less studied. Under certain conditions, the heteroepitaxy of Ge on Si (001) can produce quantum dots¹¹ as small as 8 nm in diameter with density as high as 5×10^{11} cm⁻², which is very important for technological applications both for electronic memories and for optoelectronic devices. Ge Stranskii-Krastanov islands have been studied by several experimental techniques, such as tunnelling,¹² Raman scattering,¹³ photoluminescence,^{11,14,15} admittance spectroscopy¹⁶ and capacitance spectroscopy,^{17,18} but little is known so far about their electronic spectrum and no work has been done on their transport properties.

In the present paper we study hopping conduction in modulation-doped structures, in which Ge dots are embed-

ded in the vicinity of a hole channel. The devices were formed into field-effect transistors, allowing one to control the hole concentration both in the impurity band of *p*-doped layer and in the quantum dots. We demonstrate that trapping of holes by Ge dots strongly affects the activation energy of hopping in the impurity band. We observe drain conductance modulation with respect to gate voltage due to injection of holes into quantum levels of dots and hopping transport between them.

II. EXPERIMENTALS DETAILS

The samples were fabricated on an *n*-Si (001) substrate with resistivity of 7.5 Ω cm by molecular beam epitaxy. Figure 1 shows the structure and its corresponding band diagram. After preliminary chemical processing, the substrates were placed in the growth chamber where they were cleaned at 800 °C in a weak Si flux. As a result of the cleaning process, an atomically pure surface with a (2 \times 1) superstructure is formed. Next, a 100-nm *i*-Si buffer layer, a 40-nm *p*-Si layer (3×10^{17} cm⁻³ B with a degree of compensation $K < 3 \times 10^{-3}$) and another 40-nm *i*-Si layer were grown at 500 °C. After that the Ge layer was deposited at 300 °C at a rate of 0.3 ML/s (1 ML=1.4 Å). The nominal Ge thickness, d_{eff} , was varied from 0 ML (no Ge) to 20 ML along the wafer diameter by step-by-step movement of a shutter inserted into the Ge beam during the growth process. The structure was finally capped with 40 nm of *i*-Si. The doped Si layer serves as a source of holes which can be absorbed by the potential well in the valence band of the Ge QD's. Al source and drain electrodes were deposited on top

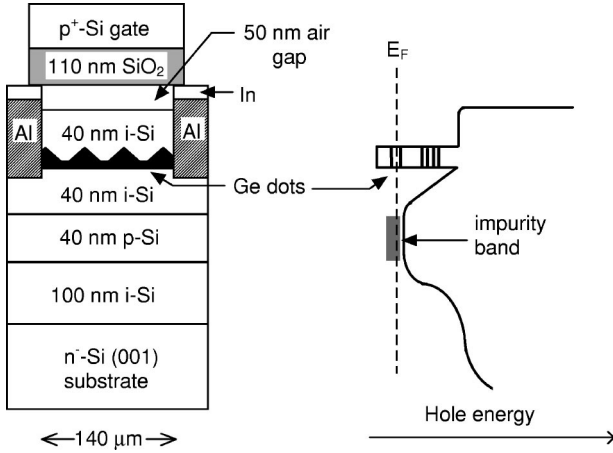


FIG. 1. Schematic diagram of the sample structure, and its valence band diagram.

of the structure and heated at 450 °C in a N₂ atmosphere to form reproducible ohmic contacts, followed by evaporation of thin (~10 nm) indium strips. The spacing between source and drain was 140 μm with a channel width of 3 nm.

Due to its ~4% lattice mismatch with respect to the Si, the Ge layer starts to grow commensurately until a critical thickness is reached, when islands are formed spontaneously. For present growth conditions, the critical thickness is about 4–6 ML. By this process it is possible to fabricate, coherent with the substrate, Ge nanocrystals (“hut” clusters) which have lateral dimensions of several nanometers and good size uniformity. STM studies have shown^{17,18} that for nominal Ge thickness of 10 ML, the average in-plane diameter and height of the dots are 13 and 2.5 nm, respectively. They fluctuate within a 20% range. The density of the dots is $n_{\text{QD}} = 3 \times 10^{11} \text{ cm}^{-2}$. At $d_{\text{eff}} > 13 \text{ ML}$, misfit dislocations release the strain and the structure becomes dislocation rich with huge islands having the Ge lattice constant.

For field-effect measurements, samples were prepared in the form of metal-oxide-semiconductor field-effect transistors (MOSFET’s). It was necessary to avoid sample heating above 550 °C which would cause Ge segregation. However, it was very undesirable to use low-temperature process of insulator growth because of the low dielectric breakdown threshold in such insulators. For these reasons we used a kind of “bonding” technique. A thin degenerate Si wafer (gate) was oxidized at 1000 °C in an O₂ atmosphere to produce a 110-nm-thick SiO₂. Then this gate with the oxide film was attached to the In strips of the sample in deionized water, then taken out and heated at 180 °C to “solder” the two together. The largest potential that could be applied between the gate and channel in these structures, set by dielectric breakdown, was 30 V. Special care was taken to select devices without dust particles and other contamination between oxide and sample.

We used a Keithley 6517A electrometer for measurements of the channel resistance. The source-drain voltage was fixed at 100 mV which ensures Ohmic conduction in the temperature range from 300 to 4 K. In the field-effect experiments, the gate voltage (from –25 V to +25 V) was supplied by an HP E3631A Triple Output DC Power Supply. The magnetoresistance was measured by applying a mag-

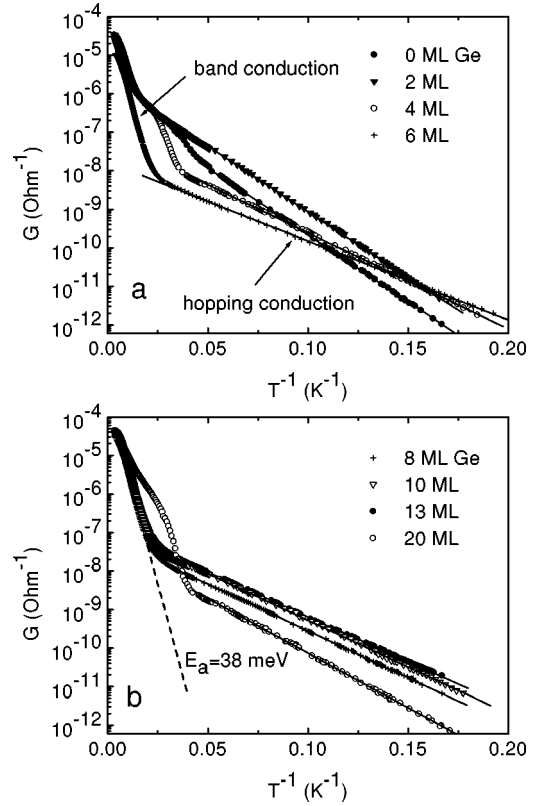


FIG. 2. Temperature dependence of conductance for various nominal thicknesses of Ge layer. The gate voltage is 0 V.

netic field perpendicular to the sample surface in the range from 0 to 1 T.

III. RESULTS AND DISCUSSION

A. Temperature dependence of conductance

The layer conductance in a series of samples where the average thickness of the Ge layer is varied is shown in Fig. 2 as a function of temperature. At temperatures above 30 K, all samples show simple activation-type characteristics with activation energy $E_a = 38\text{--}40 \text{ meV}$. This value is close to that reported for the ionization energy of an isolated B impurity state ($E_i = 45 \text{ meV}$). Some difference between E_a and E_i can be attributed to the formation of the impurity band with Coulomb potentials from the randomly-distributed charged impurity centers in the *p*-type channel (Fig. 3). If the degree of compensation tends to zero, then $E_a = E_i - 0.99e^2N_B^{1/3}/(4\pi\epsilon\epsilon_0)$, where e is the electronic charge, ϵ is the relative permittivity, and N_B is the boron concentration.¹⁹ For $N_B = 3 \times 10^{17} \text{ cm}^{-2}$, the above relation yields $E_a = 37 \text{ meV}$. Therefore, the temperature dependence of conductivity above 30 K is consistent with conduction by holes thermally activated from the impurity states to the valence band of the *p*-type Si layer.

At $T < 20\text{--}30 \text{ K}$, activated behavior is also presented but the value of the low-temperature activation energy W is much smaller than that at high T . This temperature dependence is characteristic of nearest-neighbor hopping conduction in the impurity band. Figure 3 shows W obtained from the slopes of $\ln G$ vs T^{-1} as a function of Ge coverage. One can see that hopping energy is strongly affected by the prox-

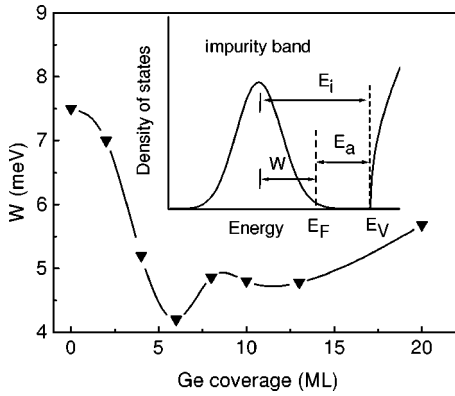


FIG. 3. Dependence of the hopping activation energy on Ge coverage. The inset shows the density of impurity states in the p -type Si band gap for a weak compensation.

imity of Ge layer when d_{eff} exceeds 2 ML, indicating that the quantum dots are the main source of hopping energy change. In the case of weak compensation, the Fermi level lies in the tail of the density of impurity states (Fig. 3). The activation energy, W , is determined by the energy difference between E_F and the center of the band. For $K \rightarrow 0$, $W = 0.99e^2N_B^{1/3}/(4\pi\epsilon\epsilon_0)$.¹⁹ If we take the experimental value of W for the bare sample (0 ML of Ge) $W = 7.5$ meV we obtain $N_B = 2.5 \times 10^{17} \text{ cm}^{-3}$ which is close to the value expected from the growth conditions. Thus, this hopping conduction channel is also associated with the p -Si layer.

We believe that the quantum dots act as controllable compensation centers by extracting holes from the impurity band. The dependence of W on K should be of the form $W = e^2N_B^{1/3}F(K)/(4\pi\epsilon\epsilon_0)$, where F is some universal function of K . It follows from the theory¹⁹ that an increase in K from 0 to 1 causes the function $F(K)$ to fall rapidly, pass through a minimum at $K_{\text{min}} \approx 0.3$ and then to rise again following the movement of the Fermi level through the impurity band. We see that similar behavior is observed in our samples (Fig. 3). At the minimum, the theory predicts $W(K_{\text{min}}) \approx 0.7W(K=0)$ which gives $W_{\text{min}} \approx 5$ meV for our case and is in agreement with the data in Fig. 3. Taking the degree of compensation at the minimum as about 0.3, we can estimate how many holes have been captured by QD's. This simple calculation yields the reasonable value of $3.6 \times 10^{11} \text{ cm}^{-2}$. Comparing with the density of quantum dots, $n_{\text{QD}} \approx 3 \times 10^{11} \text{ cm}^{-2}$, we deduce that at the minimum (about 6 ML) each dot traps about one hole.

B. Field effect

The change in channel conductance with gate voltage is shown in Fig. 4. Conductance increases at negative V_g as would be expected from the p -type nature of the material. Two important features are observed. First, the field effect is reduced by embedding the QD layer. Second, in samples which contain well-defined dots (8–13 ML¹⁷), contributions to the conductance appear which oscillate with gate voltage. The distance between successive conductance peaks, ΔV_g , depends on the average Ge thickness, in particular ΔV_g decreases with increasing QD size. At high temperatures, the peak width widened and oscillations disappeared (Fig. 5).

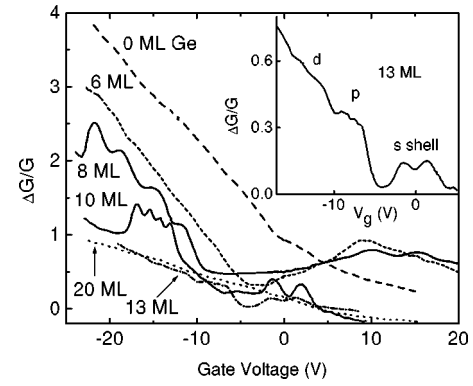


FIG. 4. Field effect at 6 K for various Ge coverages. Curves for 0, 6, and 8 ML are shifted up by 0.6 for clarity. Data are normalized on G (4 V). The inset shows an expanded view on the $G-V_g$ characteristic of the 13 ML sample.

We attribute the oscillating component to conduction by direct hopping of holes between dots, whereas the smooth background arises from accumulation of holes in the impurity band of the p -Si layer. In these samples, the dots typically have diameters of 13 nm and spacing of 10 nm so the separation between them is 3–4 nm.¹⁷ This is a reasonable distance for tunnelling in the silicon and is compatible with the presence of variable-range hopping in the quantum dot layer.

Applying the gate potential induces a charge into the system with density given by $\Delta\sigma = C_{\text{gate}}V_g$, where C_{gate} is the capacitance per unit area between gate and film. This results in filling of the dots by holes. Since the density of states in the QD's is discrete, the change of dot occupation gives rise to distinct features in the $G-V_g$ traces. The condition for a maximum in conductance is that the corresponding level is only half filled. In the case of a fully occupied state, the hole has to be activated to the next energy level in a dot. This requires a larger activation energy, and therefore the conductance associated with this process is smaller. Thus the conductance spectrum reflects directly the hole energy spectrum in the QD's. Similar modulation of drain current has been observed by Horiguchi *et al.*⁶ in InAs QD field-effect structures using a split gate. Remarkably, in our samples, well-resolved conductance oscillations are observed in channels which contain about 10^9 dots, whereas in the InAs/GaAs system there were only 100 InAs dots between the split gate electrodes.⁶

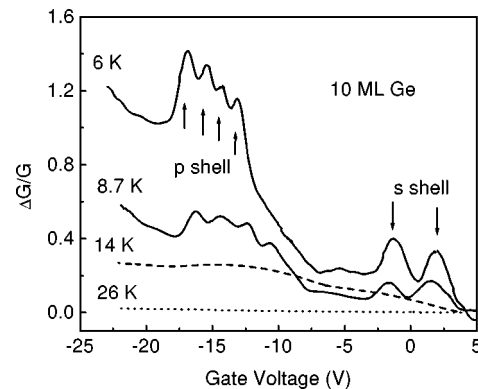


FIG. 5. Field effect for the 10 ML sample at various temperatures.

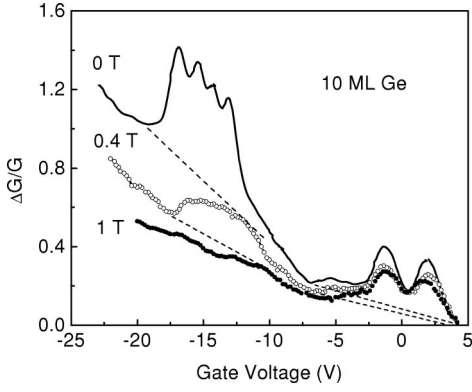


FIG. 6. Field effect for the 10 ML sample in a magnetic field at $T \approx 6$ K.

In a magnetic field, the field effect decreases (Fig. 6) corresponding to a positive magnetoresistance (MR). The most important finding is the rapid disappearance of the conductance oscillations. This is seen more clearly at high V_g , where higher states in QD's are occupied. It is less pronounced for the low energy states around $V_g \approx 0$. An exponentially large positive MR is a characteristic feature of hopping conduction. It arises from shrinkage of the wave functions in a direction transverse to the magnetic field orientation and is therefore very sensitive to the localization radius, l . The obvious difference between the behavior of the conductivity oscillations in a magnetic field for excited states and for the ground state results from the difference in their spatial dimensions. For a weak magnetic field [$l < L_B$, where $L_B = (\hbar/eB)^{1/2}$ is the magnetic length], the conductivity should decrease with the field B as²⁰

$$G(B) = G(0) \exp\{-0.04l/(L_B^4 n)\},$$

where n is the concentration of localized states. By this formula we can estimate the relation between the characteristic lengths of excited and ground states

$$l_{\text{ex}}/l_{\text{gr}} \approx \ln[G_{\text{ex}}(0)/G_{\text{ex}}(B)]/\ln[G_{\text{gr}}(0)/G_{\text{gr}}(B)],$$

where G_{gr} and G_{ex} are conductances of the QD's layer at low V_g and at high V_g , respectively, when the ground and excited states are occupied. To obtain the "pure" contribution from the QD's we must subtract the background as indicated by the dash lines in Fig. 6. Taking the data at $V_g = -1.2$ V as G_{gr} and at $V_g = -15$ V as G_{ex} , from their change in a field of 0.4 T, $G_{\text{ex}}(0 \text{ T})/G_{\text{ex}}(0.4 \text{ T}) = 3.5$ and $G_{\text{gr}}(0 \text{ T})/G_{\text{gr}}(0.4 \text{ T}) = 1.5$ we obtain $l_{\text{ex}}/l_{\text{gr}} \approx 3$ which is reasonable.

For the 8 and 10 ML samples, the conductance structure reveals two distinct shells of the hole states in the Ge QD's. The first shell contains two peaks, the second displays four well-pronounced maxima (see for example Fig. 5). This structure can be explained well by the model which assumes a two-dimensional parabolic lateral confinement in the dots.²¹ At zero magnetic field, the energy-level diagram consists of equidistant states $E_{n,l} = (2n + |l| + 1)\hbar\omega$, where $\hbar\omega$ is the quantization energy and l is the angular momentum number.²² The degeneracy of a state with energy $(m + 1)\hbar\omega$ is $2(m + 1)$ with $m = 2n + |l|$. For $n = 0$, the s -like ground state ($l = 0$) can accommodate only two holes. The

p -like first excited state ($l = \pm 1$) has a twofold orbital as well as twofold spin degeneracy. However, the degeneracy of the states is lifted by electron-electron interaction in the dots. So the difference in the gate voltage between loading of the $(N - 1)$ th and N th holes into the same shell is a direct consequence of Coulomb repulsion. In the 13 ML sample, one more broad shoulder can be identified around $V_g \approx -13$ V (see inset in Fig. 4). We associate it with charging of the second excited d -like state ($l = \pm 2$). Unfortunately, the individual charging peaks of the d shell are not resolved due to inhomogeneous broadening in the dot ensemble. One can see in Fig. 4 that, at zero gate bias, the dots are charged by one or two holes only, which is consistent with the discussion of the compensation role of the QD's.

The energy level separation (ΔE) of the different charge states in the dots can be estimated by using $\Delta E = \eta e \Delta V_g$, where the gate modulation coefficient η relates the gate voltage to the hole energy inside the dot. This coefficient can be determined from the following electrostatic considerations. Since the field effect is strongly reduced with increasing dot density, we can assume that most of the charge, $\Delta\sigma$, induced by gate voltage is captured by the QD's. Then, the change in the charge of each dot is $\Delta q_{\text{QD}} = \Delta\sigma/n_{\text{QD}}$ and this gives rise to a change in potential of the dot $\Delta\phi = \Delta q_{\text{QD}}/C_{\text{QD}} = C_{\text{gate}}\Delta V_g/(n_{\text{QD}}C_{\text{QD}})$, where C_{QD} is the dot self-capacitance. Thus the final result is

$$\eta = \Delta\phi/\Delta V_g = C_{\text{gate}}/(n_{\text{QD}}C_{\text{QD}}).$$

Let us calculate η for the 10 ML sample. The value of C_{QD} for a disk-shaped dot with diameter D in classical electrostatics is given by $C_{\text{QD}} = 4\epsilon\epsilon_0 D$. For $D = 13$ nm and $\epsilon = \epsilon_{\text{Si}} = 11.7$, this yields $C_{\text{QD}} = 4.8$ aF. The gate capacitance consists of the capacitances of oxide film and of air gap in series. Taking the appropriate geometrical parameters of the structure (Fig. 1), $n_{\text{QD}} = 3 \times 10^{11} \text{ cm}^{-2}$ and relative permittivities 4 for SiO_2 and 1 for the air gap, we find $C_{\text{gate}} = 1.2 \times 10^{-4} \text{ F/m}^2$ and $\eta = 0.83 \times 10^{-2}$.

The gate voltage difference between the two peaks in the s shell is 3.3 V for the 10 ML sample, and hence the estimated energy gap between singly and doubly occupied states, i.e., the s - s correlation energy E_c^{s-s} , is 28 meV. This value is in reasonable agreement with the charging energy obtained in the capacitance spectroscopy experiments,¹⁷ 36 meV, and by studies of the barrier admittance,¹⁶ 29 meV. Similarly, the p states are separated by $\Delta V_g \approx 1.2$ V, giving $E_c^{p-p} \approx 11$ meV. We note that E_c^{p-p} is smaller than E_c^{s-s} by a factor of about 3. The reason is that the spatial dimension of the wave function of the excited states is larger than that of the ground state. Therefore the interaction energy, $E_c \propto l^{-1}$, gets smaller. This explanation implies $l_p/l_s \approx 3$ which agrees well with analysis of the magnetoresistance data. Similar calculations allowed us to determine the characteristic energies for the other samples, in particular for the 8 and 13 ML samples. The results are depicted in Fig. 7. It seems to be quite reasonable that all energies decrease with increasing the nominal Ge thickness due to increase of the QD's size.

We may also obtain the separation of the s and p energy levels in the dots, δ_{sp} , which, in the harmonic well approximation, equals the quantum energy $\hbar\omega$. We have to re-

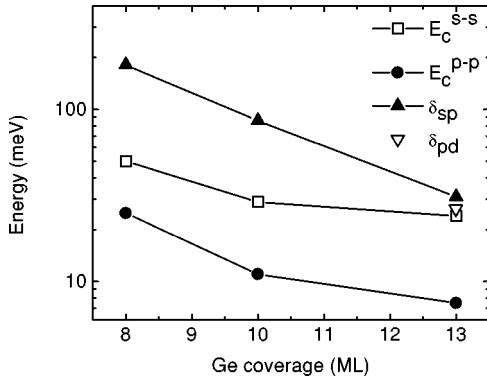


FIG. 7. Variation with Ge coverage of correlation (charging) energies in the s and p shells, E_c^{s-s} and E_c^{p-p} , and the bare level spacings, δ_{sp} and δ_{pd} .

member that in the experiments the levels are filled sequentially so that the ΔE 's include relevant correlation energies. These have to be subtracted to obtain the ‘‘bare’’ level separation

$$\delta_{sp} = \hbar\omega = \Delta E^{s-p} - 2E_c^{s-p},$$

where $\Delta E^{s-p} = 122$ meV is the energy difference between loading the first hole into the s state and the first hole into the p state. (Our value for ΔE^{s-p} agrees well with that obtained by Zhang *et al.*¹⁶ which is 125 meV.) The term $2E_c^{s-p}$ corrects for the correlation energy between the hole entering the p state and the two holes already present in the s state. We cannot independently measure E_c^{s-p} but we may obtain a rough estimate for it by using the physically obvious result

$$E_c^{s-s} > E_c^{s-p} > E_c^{p-p}.$$

Taking the geometrical mean of E_c^{s-s} and E_c^{p-p} , we use $E_c^{s-p} = 18$ meV. Applying the correction, we obtain $\delta_{sp} = \hbar\omega \approx 86$ meV which is close to the value of about 80 meV observed in resonant tunneling experiments.¹² Bare level spacings are also shown as functions of Ge coverage in Fig. 7.

From the quantum energy we may calculate the characteristic oscillator length $l = \sqrt{\hbar/(m^*\omega)}$ nm in the quantum dots. Using the effective mass for heavy holes in Ge, $m^* = 0.34m_0$, we obtain $l = 1.5$ nm. We may also estimate l from the correlation energy in the s level using the relation²³ $E_c^{s-s} = e^2/(4\pi\epsilon\epsilon_0 l)$, which leads to $l = 2.9$ nm for $\epsilon = \epsilon_{\text{Ge}} = 16$. The agreement between two above values is quite satisfactory especially if we remember that strain can modify the carrier effective mass. Also, deviation from an harmonic potential may exist.

IV. CONCLUSIONS

We have studied effects of embedded Ge dots on hole transport in modulation-doped Si-based structures. We have found that the QD's act as controllable compensation centers changing the activation energy of hopping conduction in the impurity band of the underlying p -doped Si layer. Conductance modulation, corresponding to changing the number of holes per dot, has been observed by varying the gate potential. The oscillating field effect is attributed to hopping conduction through the discrete energy levels in the dots. The correlation (charging) energies in ground and first excited states, the quantization energies and the localization lengths have been determined.

ACKNOWLEDGMENTS

This work was supported by grants from the Interdisciplinary Scientific and Technical Program ‘‘Physics of Solid State Nanostructures’’ (Grant No. 98-1100), the Intercollegiate Scientific Program ‘‘Universities of Russia, Basic Research’’ (Grant No. 4103) and the International Association for the Promotion of Cooperation with Scientists of the Independent States of the former Soviet Union (Project No. 94-4435). One of authors (A.I.Y.) gratefully acknowledges financial support from the Department of Physics (University of Cambridge) which enabled him to carry out low-temperature measurements in Cambridge. We also thank Dr. E. G. Astrakharchik for experimental assistance and the Engineering and Physical Sciences Research Council for financial support.

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