JETP Letters, Vol. 75, No. 2, 2002, pp. 102–106. Translated from Pis’ma v Zhurnal Éksperimental’noĭ i Teoreticheskoĭ Fiziki, Vol. 75, No. 2, 2002, pp. 113–117.
Original Russian Text Copyright © 2002 by Yakimov, Dvurechenskiœ, Nikiforov, Chaĭkovskiœ.

Barrier Height and Tunneling Current in Schottky Diodes with Embedded Layers of Quantum Dots

A. I. Yakimov, A. V. Dvurechenskiĭ, A. I. Nikiforov, and S. V. Chaĭkovskiĭ
Institute of Semiconductor Physics, Siberian Division, Russian Academy of Sciences,
pr. akademika Lavrent’eva 13, Novosibirsk, 630090 Russia
e-mail: yakimov@isp.nsc.ru

Received December 20, 2001

Electrical characteristics of silicon Schottky diodes containing Ge quantum dot (QD) arrays are investigated. It has been found that the potential barrier height at the metal–semiconductor contact can be controlled by introducing dense QD layers, which is a consequence of the formation of a planar electrostatic potential of charged QDs. When the applied voltage is varied, the ideality factors of Schottky barriers exhibit oscillations due to the tunneling of holes through discrete levels in quantum dots. © *2002 MAIK “Nauka/Interperiodica”.*

PACS numbers: 73.20.Mf; 73.50.Pz

The last decade has been marked with great progress of nanoelectronics. Its advances are largely associated with the introduction of nanostructures with quantum dots (QDs). QDs represent the limiting case of systems with a reduced dimensionality, because the motion of charge carriers in these systems is spatially confined to sizes smaller than the electron wavelength in all three dimensions. The dimensionality of the electron states in QDs is considered equal to zero, and quantum dots in this sense are artificial analogues of atoms [1]. The discrete energy spectrum of electron states localized in QDs serves as the characteristic feature of zero-dimensional systems that determines the particularity of physical phenomena in nanostructures with QDs [2]. A particular region of physical phenomena associated with the discreteness of the charge transferred by one electron and called single-electron processes is typical of electron transport processes in structures with QDs [3]. The attractive fact is that the characteristics of single-electron devices are universal in the sense that these are determined by only the mutual QD–drain, QD–source, and QD–gate capacitances and do not depend on the particular implementation of the diode or transistor.

Because of small sizes (~10 nm) and the high uniformity of their sizes and shape, self-organized QDs that form in the heteroepitaxy of elastically strained systems are most attractive from the practical point of view [4, 5]. Successful attempts at developing efficient heterolasers [4], photodetectors in the IR region [6], tunnel diodes [7], quantum transistors [8], and single-electron memory elements [9] based on arrays of such QDs are in progress already. A broad range of fundamental physical problems associated with revealing the mechanisms and regularities of charge transfer in device structures with embedded QD layers arise in this connection.

This work is devoted to studying the potential distribution and electron transport processes in silicon Schottky diodes containing an array of germanium nanoclusters. Ge and Si islands represent potential wells for holes and can be charged with a positive charge, capturing holes from the surrounding volume and thus changing the potential in the vicinity of the Schottky barrier. In addition, the occurrence of discrete energy states in Ge QDs can enhance processes of tunneling leakage of holes through the barrier. A knowledge of fundamental physical phenomena in such systems allows semiconductor diodes with required electrical characteristics to be developed purposefully.

The aim of this work was to find the regularities of the formation of the potential barrier and the variation of the ideality factor upon introducing QD layers into the region of the metal–semiconductor contact.

Formation of Schottky diodes with QDs. A schematic representation of a structure cross-section is shown in Fig. 1. Samples were grown by molecular beam epitaxy on phosphorus-doped Si(001) substrates with a resistivity of 7.5 Ω cm. The growth temperature of Si layers was 800 and 500°C before and after the deposition of a Ge layer, respectively. After cleaning the substrate, a Si buffer layer 50 nm thick was grown, on which a p^+-Si layer delta-doped with boron was deposited subsequently (the layer concentration of boron was 5×10^{-13} cm^{-2}). Next, a p-Si layer was grown with the boron concentration at the level $N_B \sim 5 \times 10^{-15}$ cm^{-3} and the thickness $L = 40$ nm. A Ge layer was introduced at the center of this layer at a temperature of 300°C with a varying equivalent thickness $d_{\rm eff}$. To improve the properties of the resulting metal–semiconductor interface, samples were passed through a lock into another chamber and were held in an O_2 atmosphere at a pressure of 10^{-4} Pa and a temperature of 500°C for 15 min. As a result of this procedure, a surface SiO_2 layer formed with a thickness of about 1 nm. Its role was in suppressing the formation of a static dipole layer at the interface, thus decreasing the reverse current of the diodes [10]. The ohmic contact to the buried delta-doped p^+-Si layer was formed by depositing Au followed by heating the structure at a temperature of 400°C for 10 min. The Schottky barrier was created by sputtering a Ti/Al contact on the epitaxial structure. The contact area was $A = 1.5 \times 10^{-4}$ cm^2. The samples were made in the variant of Schottky diodes with a narrow base in order to decrease the barrier height at the metal–semiconductor contact through the Schottky effect and hence to observe experimentally the change in the effective barrier height due to the electrostatic charging of QDs.

Four sets of samples were investigated. The samples of the first set did not contained Ge ($d_{\text{eff}} = 0$) and represented conventional silicon Schottky diodes. The equivalent thickness of Ge in the second set of samples comprised 5 monolayers (ML) (1 monolayer = 1.4 Å); in the third, $d_{\text{eff}} = 8$ ML; and in the fourth, $d_{\text{eff}} = 10$ ML. Under the growth conditions used in this work, a continuous Ge film grows at $d_{\text{eff}} \leq 5$ ML, and pyramidal Ge nanoclusters (QDs) faceted by {105} planes appear on the continuous film at larger thicknesses [5]. For $d_{\text{eff}} =$ 8 ML, the average size of the pyramid bases equals $a_{\text{QD}} = 10$ nm, the pyramid height is $h \sim 1.5$ nm, and the island density is 4×10^{11} cm^{-2}. For $d_{\text{eff}} = 10$ ML, these parameters are $a_{\text{QD}} = 15$ nm, $h \sim 1.5$ nm, and 3×10^{11} cm^{-2}, respectively.

Barrier height. One of the main characteristics of a Schottky diode is the potential barrier height at the metal–semiconductor interface. The potential barrier height can be found from an analysis of the temperature dependence of the I_s/T^2 ratio, where I_s is the diode saturation current and T is temperature [10]. In its turn, the saturation current can be found from a linear extrapolation of volt–ampere characteristics at $V > 3\,kT/e$ to $V = 0$ (k is the Boltzmann constant, $e = |e|$ is the absolute value of the electron charge) [10].

Figure 2 shows experimental curves of $I_s/T^2(T^{-1})$ and the barrier height φ_B determined in this way. It was found that $\varphi_B = 0.33$ eV for $d_{\text{eff}} = 0$ and 5 ML, $\varphi_B = 0.34$ eV for $d_{\text{eff}} = 8$ ML, and φ_B increases up to 0.42 eV in a sample with the equivalent thickness of Ge equal to 10 ML.

The observed growth of the barrier height can be explained based on the following model. Consider the energy diagram of a metal–p-type silicon contact (Fig. 3). The distribution of the potential due to the formation of a space-charge region (SCR) in Si along the z axis perpendicular to the growth plane is given by the equation

$$\varphi(z) = \varphi_{BS} - \frac{eN_B}{\epsilon\epsilon_0}[w(V)z - z^2/2], \qquad (1)$$

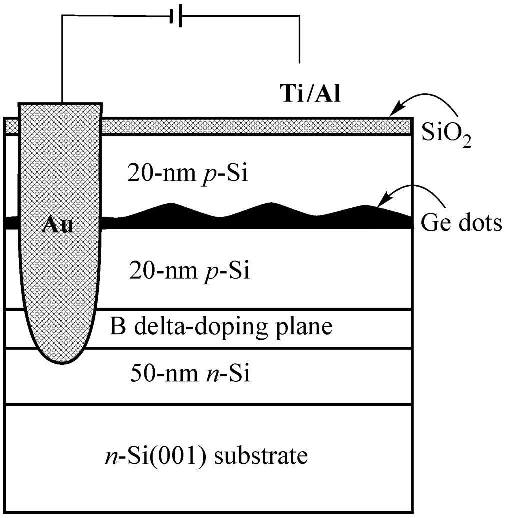

Fig. 1. Schematic representation of a cross-section of a silicon Schottky diode with Ge quantum dots.

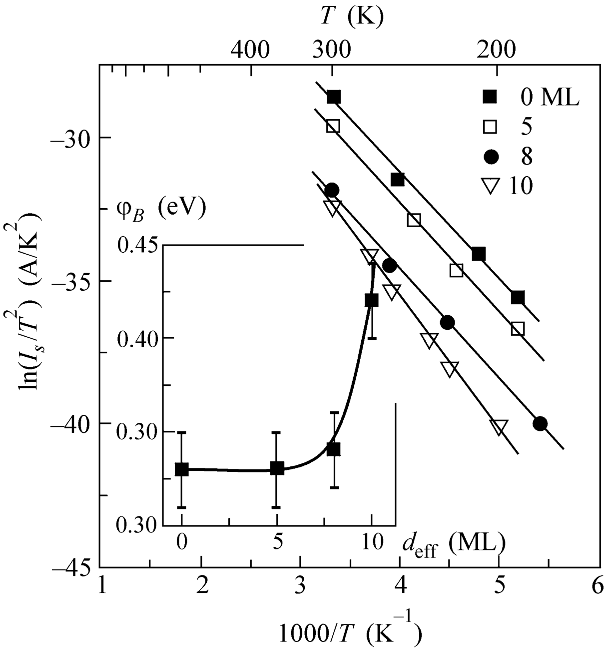

Fig. 2. Temperature dependence of the saturation current on coordinates used for determining the barrier height [10]. The inset shows the barrier height φ_B for various equivalent Ge thicknesses obtained from an analysis of $I_s/T^2(T^{-1})$ curves.

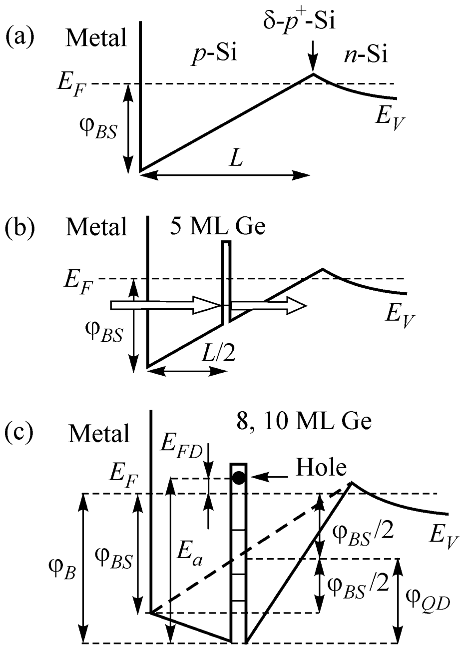

Fig. 3. Equilibrium valence band profile for a metal–p-type silicon contact along the growth direction. (a) The Ge layer is absent; (b) the Ge layer is neutral; and (c) the layer of Ge nanoclusters is charged by a positive charge of holes. E_F is the equilibrium Fermi level, φ_{BS} is the Schottky barrier height, φ_B is the effective barrier height in the presence of charged quantum dots, φ_{QD} is the change in the potential due to charged QDs, E_a is the depth of the hole energy level. The potential corresponding to the intermediate SiO_2 layer at the metal–semiconductor interface and to the buffer layer of i-Si is not shown in the figure.

where φ_{BS} is the height of the Schottky barrier, N_B is the impurity concentration, ϵ is the relative dielectric constant of Si, ϵ_0 is the electric constant, and w is the SCR width. The length of the diode base $L = 40$ nm is significantly smaller than the value of w required for the formation of a depletion layer in Si with the impurity concentration $N_B = 5 \times 10^{15}$ cm^{-3} ($w(V = 0) \approx \sqrt{(2\epsilon\epsilon_0/eN_B)(\varphi_{BS} - kT)} \approx 300$ nm); therefore, first, the boundary of the depletion layer lies in the vicinity of the delta-doped p^+-Si layer already at a zero bias and hardly shifts at the reverse bias,[1] and, second, $\varphi(z)$ is a nearly linear function (Fig. 3a). The key issue in the understanding of the effect of Ge quantum dots on the electrostatic potential in the system is the possibility of QDs accepting holes from the metal and surrounding silicon. If the thickness of the continuous germanium layer (for samples of the second set) or the sizes of Ge islands (for samples of the third and fourth sets) are so small that the size quantization levels of holes in Ge lie below the Fermi level E_F, then the Ge layer is electrically neutral and does not affect the barrier height (Fig. 3b). As the QD size increases, the hole energy level can rise above E_F and become filled with holes. In this case, the valence band edge in the plane $z = L/2$ will drop by the value φ_{QD}.

It is evident in Fig. 3c that the maximum height of the potential barrier φ_B is

$$\varphi_B = \begin{cases} \varphi_{BS}, & \text{if } \varphi_{QD} \le \varphi_{BS}/2 \\ \varphi_{QD} + \varphi_{BS}/2, & \text{if } \varphi_{QD} > \varphi_{BS}/2. \end{cases} \qquad (2)$$

In its turn, $\varphi_{QD} + \varphi_{BS}/2 = E_a - E_{FD}$, where E_a is the energy of the shallowest level of the hole-filled levels in QDs reckoned from the Si valence band edge (QD ionization energy[2]), E_{FD} is the position of the Fermi level with respect to the hole level in QDs (Fig. 3c). For QDs in which the height h is much smaller than its size in the growth plane a_{QD}, $E_{FD} \approx \pi\hbar^2\langle N\rangle/m^* a_{QD}^2$ [11], where $\langle N\rangle$ is the average number of holes in each QD, and m^* is the effective mass of charge carriers. Assuming that $a_{QD} = 15$ nm and $m^* = 0.34m_0$ for heavy holes, we obtain $E_{FD} = 2.6\langle N\rangle$ meV. In QDs of such a small size, the maximum number of holes on size quantization levels $\lesssim 10$ and the "ionization" energy is of the order of hundreds of meV [12]; therefore, $E_a - E_{FD} \approx E_a$ and $\varphi_{QD} + \varphi_{BS}/2 \approx E_a$. In this case, Eqs. (2) can be rewritten in a more demonstrative form

$$\varphi_B \approx \begin{cases} \varphi_{BS}, & \text{if } E_a \le \varphi_{BS} \\ E_a, & \text{if } E_a > \varphi_{BS}. \end{cases} \qquad (3)$$

The energy spectrum of holes in analogous layers of Ge/Si quantum dots was studied previously by photoconductivity spectroscopy [13], field-effect measurements [14], and deep level transient spectroscopy (DLTS) [15]. It was found that the ground-state energy of holes is $E_a = 0.34$ eV for Ge QDs forming at $d_{\text{eff}} = 8$ ML and $E_a = 0.40$–0.42 eV for $d_{\text{eff}} = 10$ ML. It is evident that both these values are to a good accuracy equal to the effective barrier heights φ_B determined from an analysis of the temperature dependence of the saturation current in Fig. 2.

Ideality factor. The volt–ampere characteristics of metal–semiconductor barriers are often written in the form $I = I_s[\exp(eV/nkT) - 1]$, where n is the ideality factor. At a low doping level and relatively high temperatures, n is close to unity. The deviation of n from unity in Schottky diodes is mainly associated with the occur-

---

[1] Measurements of voltage–capacitance characteristics showed that the barrier capacitance of the diodes at the reverse bias in the voltage range $0 \le V \le 1$ V is actually independent of the applied voltage and equals $\epsilon\epsilon_0 A/L$.

[2] In fact, the term "ionization energy" is appropriate in full measure only for atoms, because the removal of an electron from an atom gives rise to an ion. As a rule, the situation is opposite in QDs: QDs are neutral when they contain no conduction electrons, and QDs acquire an excess charge only when they capture electrons or holes.

rence of the tunneling current component [10]; therefore, an analysis of n provides information on tunneling processes in structures with QDs [16].

The ideality factor in the case of a reverse bias is determined by the equation [17]

$$n(V) = \frac{e}{kT}\partial V/\partial \ln\left[\frac{I\exp(eV/kT)}{\exp(eV/kT)-1}\right]. \qquad (4)$$

Figure 4 displays experimental curves of n vs. the reverse bias for various samples. As the equivalent Ge thickness increases, the ideality factor grows, and peaks appear in curves $n(V)$ at $d_{\mathrm{eff}} \geq 5$ ML, which points to a resonance character of the tunneling current. Resonance tunneling processes are a characteristic feature of charge carrier transport in double-barrier structures of reduced dimensionality and are due to the quantization of the energy spectrum of electrons or holes in the region confined between the barriers. As the reverse bias increases, the energy levels of holes in the QD layer reach in turn a resonance with the quasi-Fermi level in the metal. In this case, the probability of tunneling through the Schottky barrier and, hence, the ideality factor must increase, which is actually observed in our experiments.

A peak in curves $n(V)$ at voltages $V \simeq 1.1$ V is observed for all samples containing a Ge layer; therefore, we associate this peak with the penetration of holes through the energy level of a two-dimensional state in the continuous Ge layer (Fig. 3b), because this layer has the same thickness of 5 ML in all the samples containing Ge. The peaks at lower voltages in samples with $d_{\mathrm{eff}} = 8$ and 10 ML are due to the tunneling of holes through discrete levels in QDs lying above the energy level in the continuous Ge layer.

The period of oscillations in curves $n(V)$ is reproduced sufficiently well at various temperatures (Fig. 4b). The average period at $d_{\mathrm{eff}} = 10$ ML is $\Delta V \approx$ 160 mV. Assuming that the QD layer is introduced exactly in the middle of the diode base and neglecting the band bending due to the potential of the ionized impurity in the diode base, one can estimate the energy gap between the hole levels in Ge nanoclusters at $\Delta E \approx e\Delta V/2 \approx 80$ meV. This value is in a reasonable agreement with the value of the energy gap between size quantization levels of holes in analogous Ge QDs (70–75 meV) determined by IR absorption [18] and resonance tunneling in p^+–i–p^+ structures [2].

In conclusion, it is important to note that the potential barrier height in structures with QDs can be increased only in the case of sufficiently dense packing of QDs in the layer. Otherwise, the array of charged QDs will not form a uniform planar barrier, which could efficiently control the transport of holes through the structure. In a sense, the phenomenon of a change in the height of the Schottky barrier upon introducing QD layers into the system is close in mechanism to the phenomenon that takes place in the case when surface states exist at the metal–semiconductor interface. However, if the density of local levels and their energy spectrum are determined in the last case by the quality of the interface and are not controlled in practice, the parameters of QDs (their density, sizes, and spectrum of charge carrier states) are readily amenable to control at the modern technology level. This allows effective control of the electrical characteristics of devices. The phenomenon of oscillations of the ideality factor in the case of a reverse bias in Schottky diodes with QDs may serve as a basis for the development of a new method of electron spectroscopy of energy levels in systems with reduced dimensionality.

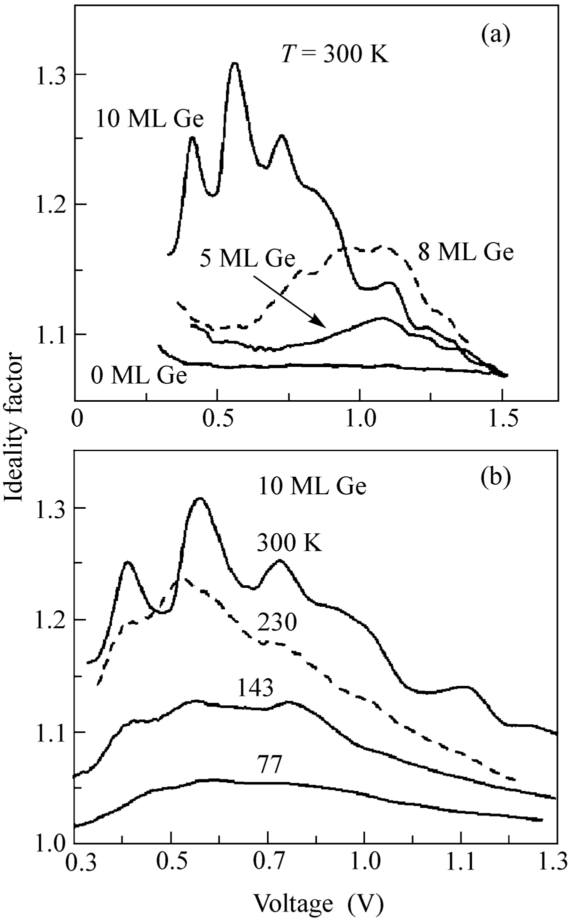

Fig. 4. Dependence of the ideality factor on the reverse bias. (a) Curves for various equivalent thicknesses of the Ge layer d_{eff} (T = 300 K). (b) Curves for various temperatures for a sample with d_{eff} = 10 ML.

The authors are grateful to V.I. Ryzhiĭ for useful discussions. This work was supported by the Russian Foundation for Basic Research, project no. 00-02-17885 and the Ministry of Education of the Russian Federation (project no. E00-3.4-154).

REFERENCES

1. L. Jacak, P. Hawrylak, and A. Wojs, *Quantum Dots* (Springer-Verlag, Berlin, 1998).
2. A. V. Dvurechenskiĭ and A. I. Yakimov, Usp. Fiz. Nauk **171**, 7 (2001).
3. U. Meirav and E. B. Foxman, Semicond. Sci. Technol. **10**, 255 (1995).
4. N. N. Ledentsov, V. M. Ustinov, V. A. Shchukin, *et al.*, Fiz. Tekh. Poluprovodn. (St. Petersburg) **32**, 385 (1998) [Semiconductors **32**, 343 (1998)].
5. O. P. Pchelyakov, Yu. B. Bolkhovityanov, A. V. Dvurechenskiĭ, *et al.*, Fiz. Tekh. Poluprovodn. (St. Petersburg) **34**, 1281 (2000) [Semiconductors **34**, 1229 (2000)].
6. A. I. Yakimov, A. V. Dvurechenskii, A. I. Nikiforov, and Yu. Proskuryakov, J. Appl. Phys. **89**, 5676 (2001).
7. O. G. Schmidt, U. Denker, K. Eberl, *et al.*, Appl. Phys. Lett. **77**, 4341 (2000); H. W. Li and T. H. Wang, Physica B (Amsterdam) **304**, 107 (2001).
8. J. Phillips, K. Kamath, T. Brock, and P. Bhattacharya, Appl. Phys. Lett. **72**, 3509 (1998); K. H. Schmidt, M. Versen, U. Kunze, *et al.*, Phys. Rev. B **62**, 15879 (2000).
9. S. Tiwari, F. Rana, H. Hanafi, *et al.*, Appl. Phys. Lett. **68**, 1377 (1996); L. Guo, E. Leobandung, and S. Chou, Appl. Phys. Lett. **70**, 850 (1997); N. Takahashi, H. Ishikuro, and T. Hiramoto, Appl. Phys. Lett. **76**, 209 (2000).
10. S. Sze, *Physics of Semiconductor Devices* (Wiley, New York, 1981; Mir, Moscow, 1984).
11. V. Ryzhii, I. Khmyrova, V. Pipa, *et al.*, Semicond. Sci. Technol. **16**, 331 (2001); V. Ryzhii, J. Appl. Phys. **89**, 5117 (2001).
12. A. I. Nikiforov, V. A. Cherepanov, O. P. Pchelyakov, *et al.*, Thin Solid Films **380**, 158 (2000).
13. A. I. Yakimov, A. V. Dvurechenskii, Yu. Proskuryakov, *et al.*, Appl. Phys. Lett. **75**, 1413 (1999).
14. A. I. Yakimov, A. V. Dvurechenskii, V. V. Kirienko, *et al.*, Phys. Rev. B **61**, 10 868 (2000).
15. N. P. Stepina, R. Beyer, A. I. Yakimov, *et al.*, submitted to Phys. Low-Dimens. Struct.
16. T. H. Wang, H. W. Li, and J. M. Zhou, Appl. Phys. Lett. **79**, 1537 (2001).
17. S. Averine, Y. C. Chan, and Y. L. Lam, Appl. Phys. Lett. **77**, 274 (2000).
18. A. I. Yakimov, A. V. Dvurechenskii, N. P. Stepina, and A. I. Nikiforov, Phys. Rev. B **62**, 9939 (2000).

Translated by A. Bagatur'yants

SPELL: OK