Size effect of parallel silicide contact

I. Ohdomari and H. Aochi
School of Science and Engineering, Waseda University, 3-4-1 Ohkubo, Shinjuku-ku, Tokyo 160, Japan
(Received 26 August 1985; revised manuscript received 16 September 1986)

When two silicides with different Schottky barrier heights coexist at a silicide-Si interface, the apparent barrier-height measured by forward I-V characteristics depends not only on the fraction of the area of the low-barrier phase but on the size of the low-barrier phase. In this study, apparent barrier heights for varying size of the low-barrier phase have been obtained by numerical analysis of both Poisson's equation and the current continuity equation. The apparent barrier height approaches the mean value of Schottky-barrier heights weighted by the low- and high-barrier areas as the size of the low-barrier phase decreases to about five times the Debye length. When the size of the low-barrier phase is of the magnitude of 500 times or more the Debye length, the apparent barrier height approaches the value determined by the fraction of the area of low-barrier phase as reported earlier [I. Ohdomari and K. N. Tu, J. Appl. Phys. 51, 3735 (1981)].

INTRODUCTION

Most of silicide-Si interfaces have very reproducible Schottky-barrier heights (SBH's) because the interfaces are independent of the condition of the original silicon surface. However, when two different phases with high and low SBH's coexist at the interface, namely, in the so-called parallel silicide contacts, the apparent SBH which is obtained from forward I-V characteristics as an average of high and low SBH weighted by the area of each phase is determined by a fraction of the area of the low-barrier phase and a combination of the two SBH's.

In our previous paper,[1] we assumed a very sharp potential distribution in Si in the vicinity of the high- and low-barrier interface as shown in Fig. 1(a) and found that even a small fraction of the area of the low-barrier phase can reduce the apparent SBH. The result was confirmed by a model experiment in which two discrete high- and low-barrier diodes were used.

Afterwards, Freeouf *et al.* pointed out that the average SBH in the parallel silicide contacts is not so sensitive to the fraction of the low-barrier phase when the size of the low-barrier phase is not much larger than Debye length.[2] This was the first work to predict the size dependence of effective barrier heights of the parallel contacts. They have shown, by using a finite element device analysis program, that as the low-barrier-height region width gets smaller, it is more effectively pinched off by the large-barrier contact, leading to a larger barrier.

This work, however, has used a specialized boundary condition at the high- and low-barrier interface in order to use the device analysis program with fixed area ratios.

For a more comprehensive understanding of the size dependence, we have calculated the following.

(i) Potential distribution in the Si substrate of the parallel silicide contact under the boundary condition at the interface which is solved sequentially in the process of the calculation. (ii) Apparent barrier height using the above potential distribution.

The calculation has been done for the low-barrier region greater than the Si Debye length. Our very important finding is that the apparent SBH is strongly influenced by the size of low-barrier phase even when the fraction of the area is same.

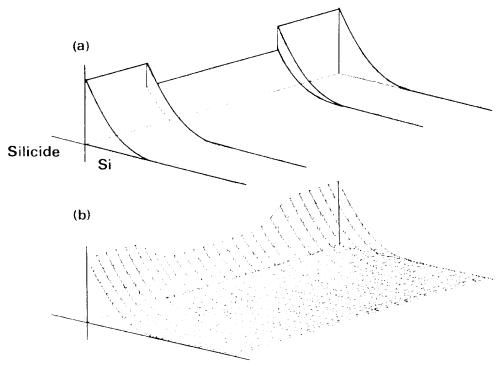

FIG. 1. Two-dimensional potential distribution in Si of parallel contacts (a) for the case where continuity of electrostatic field is ignored. (b) Result of present work.

METHOD OF CALCULATION

When continuity of the electrostatic field is neglected, potential distribution in Si can be drawn as shown in Fig. 1(a). In the actual situation, since space-charge distributions of the two barriers are different, carrier diffusion from the higher side to the lower side occurs and a new electrostatic field comes into existence. The new field takes a part of stopping power to further carrier diffusion, and thermal equilibrium is finally reached. The equilibrium potential distribution is shown in Fig. 1(b). Since a metal Debye length is an order of a few Å and is much smaller than the Si Debye length, the influence of the

metal Debye length on the potential distribution along radial direction is negligible.

To simulate this event, both Poisson's equation and current continuity equation must be solved simultaneously. Generally this is a very difficult problem. However, if the approximation that the carrier density in the conduction band of thermal equilibrium takes a Boltzmann distribution holds, the continuity equation is automatically satisfied. This approximation is reasonable when donor concentration in Si (N_d) is less than 10^{18} cm^{-3}. Schottky contacts are usually made on a high-resistivity Si substrate. So we have only to find a solution of Poisson's equation.

For calculation, we have used a model parallel contact where a low-barrier phase takes a circular form surrounded by a high-barrier phase and in contact with a Si substrate, as shown in Fig.2. The region of calculation is shown as the hatched area. Using this model, Poisson's equation is expressed as follows with two-dimensional cylindrical coordinates.

$$\left[\frac{1}{r}\frac{\partial}{\partial r}+\frac{\partial^2}{\partial r^2}+\frac{\partial^2}{\partial z^2}\right]\phi(r,z) = -\frac{e}{\epsilon}N_d\left[1-\exp\left[\frac{e}{kT}\phi(r,z)\right]\right] . \quad (1)$$

Here ϵ is the permittivity of Si.

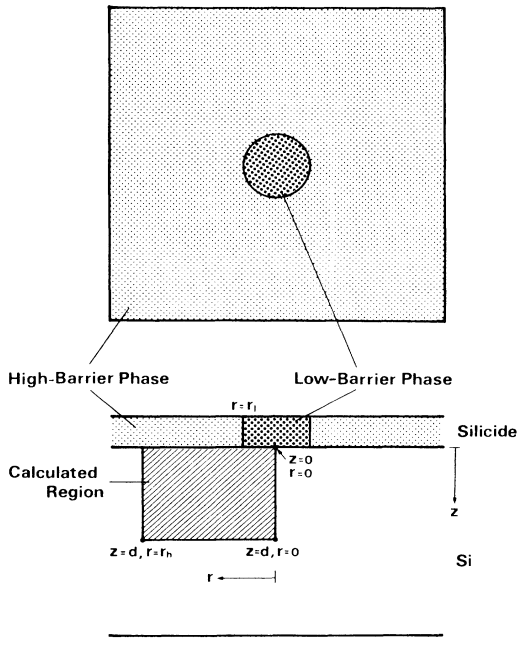

FIG. 2. Planar and cross-sectional view of the model for simulation. The region for calculation is demonstrated by the hatched area.

A procedure of the calculation is a general method of successive approximation of the difference equation transformed from Eq. (1) combined with Newton's method. Figure 3 shows the orientation of the discrete variables. Minute depth dz and minute radius dr are approximated as Δz and Δr, respectively. Therefore, each point (z,r) in the calculated region is expressed by $(i\,\Delta z, j\,\Delta r)$ (here $i=0,1,2,\ldots$; $j=0,1,2,\ldots$). In Fig. 3, the potential at (z,r) is demonstrated as $\phi(i,j)$.

Three boundary conditions are given from the problem immediately as follows:

$$\phi=0 \quad (z=d) ,$$
$$\frac{\partial\phi}{\partial r}=0 \quad (r=0) , \quad (2)$$
$$\phi=\phi_h(z) \quad (r=r_h) .$$

Here d is the depth in Si that is much larger than the width of the depletion region (about 20 times the Debye length), r_h is the radius at which the high-barrier phase is not influenced by the low-barrier phase, and $\phi_h(z)$ is the one-dimensional SBH of the high-barrier phase. The third condition holds for the following reason. We choose the region of the high-barrier phase large enough so that at the edge of the region ($r=r_h$) carriers do not move at all, hence the SBH at $r=r_h$ keeps the value of the high-barrier phase.

The two-dimensional second-order partial differential equation requires four boundary conditions or four physical conditions. Three of them are given by Eq. (2). The other boundary condition is the SBH at $z=0$ which must be defined successively in the process of calculation. Therefore, we have adopted the initial values of the successive approximation, namely, the SBH's before the charge transfer, as shown in Fig. 1(a). They are defined as follows:

$$\phi(r,z)=\begin{cases}\phi_l(z) , & r<r_l) ,\\ \phi_h(z) , & r>r_h) .\end{cases} \quad (3)$$

Here r_l is the radius of the low-barrier phase. Thus the four physical conditions are all given.

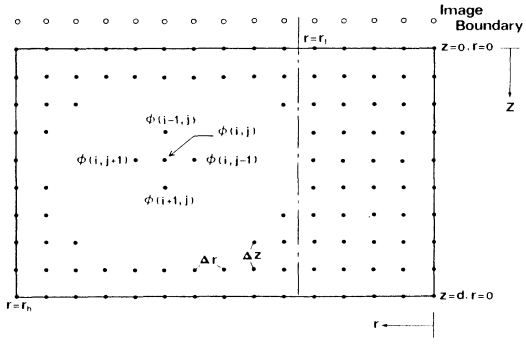

FIG. 3. Orientation of discrete variables in the calculated region shown in Fig. 2.

The values at $z=0$ must be defined with those of internal points of the calculated region by the backward difference approximation. On the other hand, the internal values of the calculated region are decided by the central approximation. The values at $z=0$ are the solution to be obtained by the present calculation, so it is better to define these with the central approximation in a similar way as for the internal values. To do this, we have made an "image boundary" outside of the real boundary at $z=0$, as shown in Fig. 3, and the values of the image boundary are decided by the backward difference approximation of the one-dimensional Poisson's equation using the values at $z=0$ and $z=\Delta z$ of the previous calculation step. The reason we use the one-dimensional equation is that the solutions diverge when the backward approximation of the two-dimensional equation is used.

With this method, we have simulated the potential distribution on the Si side of the parallel contact when N_d is 10^{17} cm^{-3}, varying the radius of the low-barrier phase and the combination of low and high SBH's.

RESULTS AND DISCUSSION

The outline of the two-dimensional potential distribution in Si is shown in Fig. 1, where r_l is 100 times the Debye length, the high SBH is 0.8 eV, and the low SBH is 0.5 eV. Figure 1(a) shows a shape for the case where carrier transfer is ignored (namely, initial values of simulation) and Fig. 1(b) shows the result of calculation. Modification of the shape appears at the boundary of the two phases.

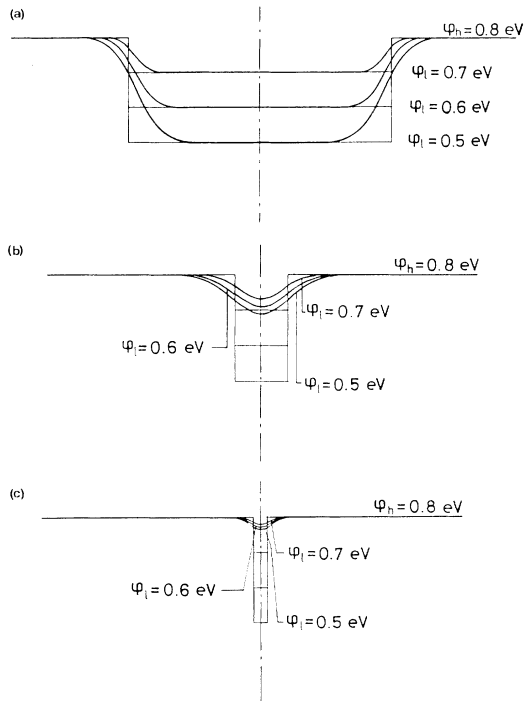

FIG. 4. Potential distribution at the silicide-Si interface, for the case where the high SBH is 0.8 eV and the low SBH is 0.7, 0.6, and 0.5 eV. (a) The radius of the low-barrier phase is (a) 100 times (b) 15 times, and (c) 3 times the Debye length.

Figure 4 shows the potential distribution at the interface, where the high SBH is 0.8 eV and the low SBH is 0.5, 0.6, and 0.7 eV. The results of simulation are shown by thick lines and initial values of calculation by thin lines. When the r_l is 100 times the Debye length [shown in Fig. 4(a)], modification is recognized only at the boundary of the two phases. When it is 15 and 3 times [shown in Fig. 4(b) and 4(c), respectively], however, the tail of the high barrier raises the bottom of the low barrier, and the effective SBH of the low-barrier phase increases.

To compare the result with our previous result,[1] the apparent SBH of the parallel contact has been evaluated on the basis of the potential distribution shown in Fig. 4. Only the thermionic emission current has been considered and the total current I has been obtained as follows by summing the component dI which passes through the minute areas of the parallel contacts:

$$I=\int_S dI \ ,$$

where

$$I=SA^{**}T^2\exp\left[-\frac{e\phi_a}{kT}\right]\left[\exp\left[\frac{eV}{kT}\right]-1\right] \ , \tag{4}$$

$$dI=A^{**}T^2\exp\left[-\frac{e\phi(r)}{kT}\right]\left[\exp\left[\frac{eV}{kT}\right]-1\right]2\pi r\,dr \ ,$$

and

$$S=\int_0^{r_h}2\pi r\,dr=\pi r_h^2 \ .$$

Here A^{**} is Richardson's constant (112 A cm^{-2}K^{-2}) and V is the applied voltage. Then it is easily shown that

$$\pi r_h^2\exp\left[-\frac{e\phi_a}{kT}\right]=\int_0^{r_h}2\pi r\exp\left[-\frac{e\phi(r)}{kT}\right]dr \ , \tag{5}$$

$$\phi_a=-\frac{kT}{e}\ln\left[\frac{2}{r_h^2}\int_0^{r_h}r\exp\left[-\frac{e\phi(r)}{kT}\right]dr\right] \ ,$$

where ϕ_a is the apparent barrier height.

In this analysis, we have neglected a contribution of recombination current and also image force lowering because the recombination current can be separated out from the $I-V$ measurement data, using a computer curve fitting to obtain the SBH value, so that the SBH is determined only on the basis of the thermionic emission theory.

Using Eq. (5), we have plotted curves ϕ_a as a function of the fraction of the area of the low-barrier phase S_l/S in Fig. 5, where the high SBH is 0.8 eV and the low SBH is 0.5 eV. The parameter is a radius of the low-barrier phase normalized by the Debye length. The insets are the schematic view of the interface structure with 10% of the

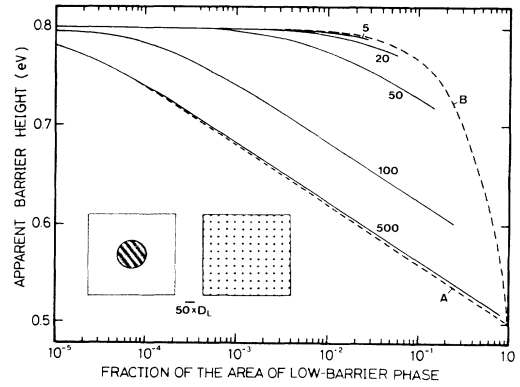

FIG. 5. Apparent SBH as a function of the fraction of the area of the low-barrier phase. The parameter is the radius of the low-barrier phase normalized by Debye length. Insets are schematic illustrations of the interface structure of parallel contacts for the case where the radius of the low-barrier phase is 100 and 5 times the Debye length.

fraction of the area of the low-barrier phase. The area of the hatched circle in the left panel equals the sum of the area of the small dots in the right panel. The radius of the hatched circle and the small dots are 100 and 5 times the Debye length, respectively. In spite of the equal fraction of the area of the low-barrier phase, it is clearly seen in the figure that the smaller size of the low-barrier phase has less influence on the apparent SBH.

When the size is larger than 500 times the Debye length, the apparent SBH approaches a limit which is given in our previous paper.[1] In this case, the apparent SBH is given by the following equation:

$$\phi_A = -\frac{kT}{e}\ln\left\{\frac{S_l}{S}\left[\exp\left[-\frac{e\phi_l}{kT}\right]-\exp\left[-\frac{e\phi_h}{kT}\right]\right]+\exp\left[-\frac{e\phi_h}{kT}\right]\right\}. \quad (6)$$

Here S_l/S is the fraction of the area of the low-barrier phase, and ϕ_l and ϕ_h are low and high SBH's, respectively. The dashed line A shows the relation of Eq. (6).

When the size of low-barrier phase is less than 5 times the Debye length, the apparent SBH approaches the other limit, the weighted mean of each SBH of two phases. This limit is given by the following equation:

$$\phi_B = \frac{S_l\phi_l + S_h\phi_h}{S}. \quad (7)$$

The dashed line B shows this relation.

This assumption is equivalent to assuming that when the high- and low-barrier phases are mixed in an atomic scale, e.g., forming an alloy, the overall work function of the alloy is given as follows, as a weighted average of each work function with composition x:

$$\phi_x = x\phi_A + (1-x)\phi_B. \quad (8)$$

The fact that the highest curve in Fig. 5 approaches the curve from the above equation clearly shows that our boundary condition is good enough for the present calculation. Actually, in some alloys, linear dependence of work functions on composition is reported.[3] Thomas and Terry have reported that when NiSi and PtSi are formed in NiPt alloy films on n-type Si with varying concentrations of Ni and Pt, the SBH of the alloy film increases linearly from that of NiSi-nSi to PtSi-nSi, corresponding to the weight percent of the Ni atom in the alloy.[4]

Zur *et al.* reported that the full depletion width is decided by the metal screening width when the metal thickness is on the order of angstroms.[5] As is described above, however, since in our calculation the lateral dimension of the low-barrier region is about a semiconductor Debye length at the smallest, the vertical size is reasonably assumed to be the same order, and hence the low-barrier region is regarded as bulky.

In Fig. 5, the apparent SBH's are not shown for the fraction of the area of the low-barrier phase close to unity. As shown in Fig. 4(c), the front of the potential distribution due to carrier transfer reaches beyond the physical boundary of the low and high barriers. Therefore, when the fronts of neighboring potential hollows overlap at a fraction of the area of the low-barrier phase, the aforementioned two-dimensional calculation becomes invalid.

To see results shown in Fig. 5 more clearly, we demonstrate in Fig. 6 the apparent SBH's as a function of the radius of the low-barrier phase normalized by Debye length with the fraction of the area of the low-barrier phase as a parameter. Here ϕ_A and ϕ_B are the SBH's calculated from Eqs. (6) and (7), respectively, and each apparent SBH is normalized by $\phi_B - \phi_A$. When the size of the low-barrier phase is smaller than 5 times the Debye length, the apparent SBH is close to ϕ_B. As the size of the low-barrier phase becomes larger, the boundary region with graded potential distribution shrinks relatively and the SBH given by Eq. (6) is finally obtained. The range of radius where the drastic decrease in the apparent SBH is

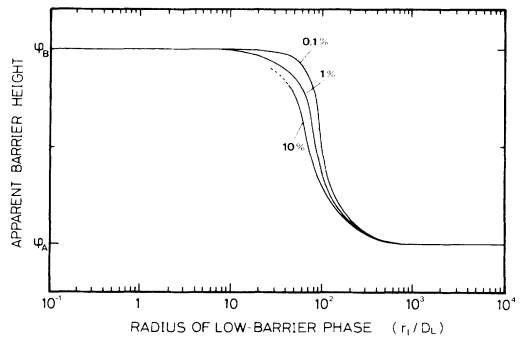

FIG. 6. Apparent SBH as a function of the radius of the low-barrier phase normalized by Debye length. The parameter is the fraction of the area of the low-barrier phase.

seen is between 20 to 100 times the Debye length, depending slightly on the fraction of the area of the low-barrier phase.

CONCLUSION

We have calculated the potential distribution on the side of the Si substrate of the parallel contact structure where two different Schottky-barrier heights coexit, and have drawn the following conclusions.

(i) The apparent SBH of parallel contacts depends on a combination of low and high SBH's, the fraction of the area of the low-barrier phase, and also the size of the patches of the low-barrier phase. (ii) The effect of the low-barrier phase decreases as the size becomes smaller. When the radius of the low-barrier phase is larger than 500 times the Debye length, the apparent SBH approaches the value which is obtained assuming no carrier transfer from the high- and to the low-barrier phase. When the radius is less than 5 times, it becomes the weighted mean of the SBH of the two phases.

ACKNOWLEDGMENT

The authors express their sincere thanks to Dr. King-Ning Tu of IBM Thomas J. Watson Research Center (Yorktown Heights, NY) for his suggestion to do this work.

[1]I. Ohdomari and K. N. Tu, J. Appl. Phys. **51**, 3735 (1981).
[2]J. L. Freeouf, T. N. Jackson, S. E. Laux, and J. M. Woodall, J. Vac. Sci. Technol. **21**, 570 (1982).
[3]A. Kiejna and K. F. Wojciechowski, J. Phys. C **16**, 6883 (1983).
[4]S. Thomas and L. E. Terry, J. Appl. Phys. **47**, 301 (1975).
[5]A. Zur, T. C. McGill, and D. L. Smith, Phys. Rev. B **28**, 2060 (1983).