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# Study of reaction and electrical properties at Ti/SiGe/Si(100) contacts for ultralarge scale integrated applications

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Solid-phase reaction, Schottky barrier heights and contact resistivities at the interface of Ti/Si<sub>0.8</sub>Ge<sub>0.2</sub>/Si(100) systems have been investigated. At annealing temperatures below 300 °C, Ti atoms preferentially react with Si atoms. Ge atoms start to react with Ti above 400 °C and C54-Ti(Si<sub>1-y</sub>Ge<sub>y</sub>)<sub>2</sub> with a fraction of  $y=0.12$  is formed by annealing at 650 °C. The annealing behavior of Schottky barrier heights suggests that the Ge composition of SiGe layers at the interface is Si-rich, which is consistent with the results on the interfacial reaction. For both  $n$ - and  $p$ -SiGe, the Schottky barrier heights lower than those of Ti/Si(100) are obtained at 650 °C, which is considered to be related to the reaction product such as C54-Ti(Si<sub>1-y</sub>Ge<sub>y</sub>)<sub>2</sub>. The contact resistivities smaller than those expected from the Schottky barrier heights are obtained for  $p^+$ -SiGe at 580 °C. The sheet resistance of Ti/Si<sub>0.8</sub>Ge<sub>0.2</sub>/Si(100) and Ti/Ge(100) systems decreases at annealing temperatures above 550 °C and the values are as small as that of C54-TiSi<sub>2</sub>. © 1998 American Vacuum Society. [S0734-211X(98)00405-3]

## I. INTRODUCTION

Due to a decrease in contact hole areas, the current driving capability of minute metal-oxide-semiconductor field-effect transistors (MOSFETs) is dominated by the parasitic series resistance of ohmic contacts with scaling-down of device dimensions.<sup>1</sup> Therefore, formation of ohmic contacts with low resistivities and high reliability is one of the key issues in ultralarge scale integrated (ULSI) circuit technologies. In the generation of 0.1  $\mu\text{m}$  rule devices, a contact resistivity lower than  $10^{-8} \Omega \text{ cm}^2$  would be necessary to maintain the performance.

We have investigated solid-phase reactions, crystallographic structures and electrical characteristics at the interfaces between various metals and Si(100) substrates and reported the low contact resistivities on the order of  $10^{-8} \Omega \text{ cm}^2$  for Zr/ and Hf/ $n^+$ -Si(100) contacts.<sup>2-5</sup> However, there are some limitations, such as the band gap, the electron affinity and the solid solubility of impurity atoms in Si, for achieving much lower contact resistivities for  $n^+$ - and  $p^+$ -Si. In particular, in complimentary metal-oxide-semiconductor (CMOS) devices, it is essentially difficult to lower the contact resistivities for  $n^+$ - and  $p^+$ -Si simultaneously by using a contact material. Since the sum of Schottky barrier heights for  $n^+$ - and  $p^+$ -Si is equal to the band gap of Si, a material with a low contact resistivity for one type of Si is disadvantageous for the other type. In addition, the maximum concentration of impurities that can be accommodated in Si at a given process temperature also limits the minimum contact resistivity. The solid solubility of B atoms in Si is lower than those of  $n$ -type impurity atoms such

as As and P. These facts suggest that the development of new contact materials is indispensable for future ULSI technologies.

From the above-mentioned viewpoint, we have tried to use Si<sub>1-x</sub>Ge<sub>x</sub> layers as intermediate layers between metals and Si substrates.<sup>6-9</sup> The application of Si<sub>1-x</sub>Ge<sub>x</sub> layers to ULSI contact systems offers many advantages such as: (1) good compatibility with Si processes, (2) controllability of the band gap, (3) heteroepitaxial growth on Si(100) substrates, and (4) different doping behavior from Si. The band gap of Si<sub>1-x</sub>Ge<sub>x</sub> varies from 1.12 to 0.66 eV by increasing the Ge fraction  $x$ . The conduction band edges of Si and Si<sub>1-x</sub>Ge<sub>x</sub> are almost aligned and the band offset is mainly formed at the valence band edge at the Si<sub>1-x</sub>Ge<sub>x</sub>/Si interface.<sup>10</sup> This fact indicates that the Schottky barrier heights of metal/ $n$ -Si<sub>1-x</sub>Ge<sub>x</sub> systems are almost the same as those of metal/ $n$ -Si and, while the narrow band gap of Si<sub>1-x</sub>Ge<sub>x</sub> results in a significant lowering of Schottky barrier heights for  $p$ -Si<sub>1-x</sub>Ge<sub>x</sub>. However, only a few experimental results on electrical properties and interfacial reaction of metal/Si<sub>1-x</sub>Ge<sub>x</sub> contacts have been reported. As for impurity doping, Tokumitsu<sup>11</sup> discussed the maximum doping concentration for various semiconductors and suggested that the  $p$ -type impurity doping in Ge has an advantage over the  $n$ -type doping from the viewpoint of the correlation between Fermi-level pinning energies. A different doping behavior from Si substrates can also be expected in the case of Si<sub>1-x</sub>Ge<sub>x</sub>.

In the present article, we report the interfacial reaction and electrical properties of Ti/Si<sub>1-x</sub>Ge<sub>x</sub>/Si(100) contacts. The results obtained in this work will also be useful for contact formation in the case of Si<sub>1-x</sub>Ge<sub>x</sub> heterostructure devices.

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## II. EXPERIMENT

The substrates used were *n*- and *p*-Si(100) with resistivities of 1–3 and 0.5–0.7  $\Omega$  cm, respectively.  $\text{Si}_{0.8}\text{Ge}_{0.2}$  layers were epitaxially grown on the substrates at a growth temperature of 460 °C by molecular beam epitaxy (MBE), whose base pressure was less than  $1 \times 10^{-10}$  Torr. Si and Ge were evaporated by electron beam guns (E-guns). Sb and Ga were also doped during the growth using Knudsen cells to form *n*- and *p*- $\text{Si}_{0.8}\text{Ge}_{0.2}$  layers. The doping concentration was examined by Hall measurements. After the  $\text{Si}_{0.8}\text{Ge}_{0.2}$  growth, the substrates were dipped into a dilute HF solution ( $\text{HF}:\text{H}_2\text{O} = 1:50$ ) and rinsed in de-ionized (DI) water before setting in a metal film deposition chamber with a base pressure below  $5 \times 10^{-10}$  Torr. By this treatment, the SiGe surface was considered to be passivated by H atoms, since no trace of oxygen adsorption was detected by x-ray photoelectron spectroscopy (XPS). Ti films were deposited on the SiGe surfaces by E-guns. Crystallographic structures were examined by a thin film x-ray diffraction (XRD) apparatus using a Cu  $K\alpha$  source and chemical compositions were measured by XPS using an Al  $K\alpha$  source and Auger photoelectron spectroscopy (AES).

In order to form Schottky diodes, the *n*- and *p*- $\text{Si}_{0.8}\text{Ge}_{0.2}$  layers with a thickness of 100 nm were grown on *n*- and *p*-Si substrates, respectively. The pseudomorphic growth of  $\text{Si}_{0.8}\text{Ge}_{0.2}$  layers on Si(100) substrates was confirmed by XRD. The doping concentrations of *n*- and *p*- $\text{Si}_{0.8}\text{Ge}_{0.2}$  layers were  $1 \times 10^{17}$  and  $1 \times 10^{16}$   $\text{cm}^{-3}$ , respectively. Ohmic contacts with Si substrates were formed on the backside of substrates by Al electrodes on heavily doped diffusion layers. The Ti film thickness of samples used in electrical measurements was 150–200 nm. Current–voltage (*I*–*V*) characteristics of Schottky diodes were measured in the temperature range of 77–300 K. The value of Schottky barrier heights was determined from the temperature dependence of the *I*–*V* characteristics.

Specific contact resistivity was also measured by a four-terminal Kelvin method.<sup>12</sup> In order to form measurement devices, *n*<sup>+</sup>- and *p*<sup>+</sup>-Si diffused layers were formed on *p*- and *n*-Si substrates by thermal diffusion of P and B atoms at 1000 °C, the surface concentrations of which were  $1 \times 10^{20}$  and  $2 \times 10^{20}$   $\text{cm}^{-3}$ , respectively. The *n*<sup>+</sup>- and *p*<sup>+</sup>- $\text{Si}_{0.8}\text{Ge}_{0.2}$  layers were grown on the *n*<sup>+</sup>- and *p*<sup>+</sup>-Si diffused layers through  $\text{SiO}_2$  masks, respectively. The doping concentrations of *n*<sup>+</sup>- and *p*<sup>+</sup>- $\text{Si}_{0.8}\text{Ge}_{0.2}$  layers were  $3 \times 10^{19}$  and  $5 \times 10^{18}$   $\text{cm}^{-3}$ , respectively.

## III. EXPERIMENTAL RESULTS

### A. Interfacial reaction

Figure 1 shows XRD spectra taken from 50-nm-thick  $\text{Ti}/\text{Si}_{0.8}\text{Ge}_{0.2}/\text{Si}(100)$  samples annealed at (a) 450 and 550 °C and (b) 650 °C. Diffraction peaks from Ti crystallites are observed for as-deposited samples and these peaks disappear at an annealing temperature of 450 °C. In the case of metal/Si systems, the formation of amorphous silicide layers has been widely reported at temperatures below 500 °C.<sup>13</sup>

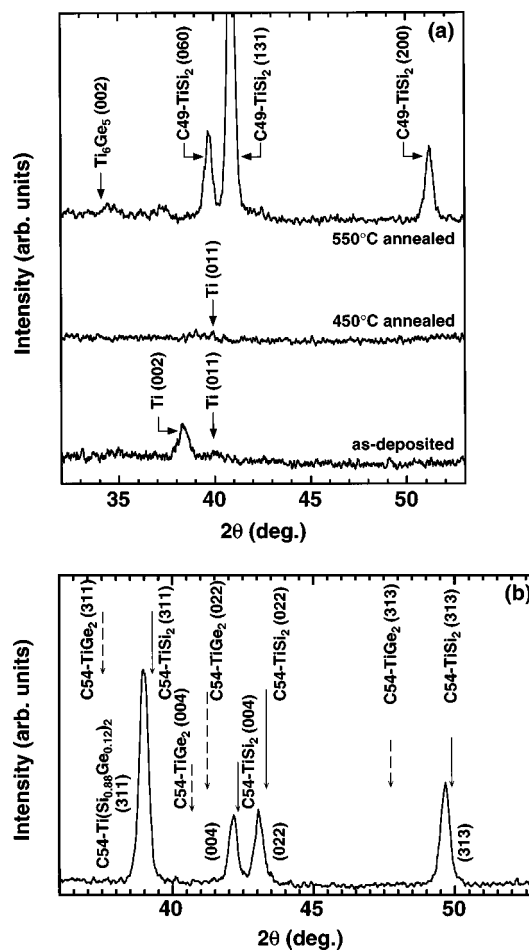


FIG. 1. XRD spectra of 50-nm-thick  $\text{Ti}/\text{Si}_{0.8}\text{Ge}_{0.2}/\text{Si}(100)$ : (a) as-deposited and annealed at 450 °C and 550 °C and (b) annealed at 650 °C.

Since the solid-phase reaction between Ti and  $\text{Si}_{1-x}\text{Ge}_x$  is considered to take place even below 400 °C as mentioned below, an amorphous layer would also be formed in this system. Distinct peaks can be observed by annealing at 550 °C. At 500 °C, we confirmed the formation of C49–TiSi<sub>2</sub> and Ti<sub>6</sub>Ge<sub>5</sub> in Ti/Si and Ti/Ge systems by XRD, respectively, which is consistent with previously reported results.<sup>14</sup> In the spectrum at 550 °C, however, the diffraction peaks from Ti<sub>6</sub>Ge<sub>5</sub> are hardly present in the case of  $\text{Ti}/\text{Si}_{0.8}\text{Ge}_{0.2}/\text{Si}$  systems and the main peaks can be assigned as the diffraction peaks originating from C49–TiSi<sub>2</sub>. This feature is considered not only to be due to the small Ge composition but also to result from the reactivity difference of Ti atoms with Si and Ge atoms, as discussed below.

At an annealing temperature of 650 °C, it should be noted that all peaks are observed between the diffraction angles expected from C54–TiSi<sub>2</sub> and C54–TiGe<sub>2</sub>, as indicated by arrows in Fig. 1(b). This result indicates that a new reaction product is formed by the reaction between Ti and  $\text{Si}_{0.8}\text{Ge}_{0.2}$  films. Boutarek *et al.*<sup>15</sup> have reported that C54–TiSi<sub>2</sub> and C54–TiGe<sub>2</sub> are completely miscible and that the lattice constant has a linear relationship with the Ge concentration. Table I indicates the lattice spacings of C54–TiSi<sub>2</sub> and C54–TiGe<sub>2</sub> and for different crystallographic planes and the

TABLE I. Lattice spacings of C54-TiSi<sub>2</sub> and C54-TiGe<sub>2</sub> for different crystallographic planes and the experimental values estimated from Fig. 2(b). The Ge fractions of Ti(Si<sub>1-y</sub>Ge<sub>y</sub>)<sub>2</sub> evaluated from the experimental results are also listed.

| hkl | Lattice spacing (Å)   |                       |              | Ge fraction: y |
|-----|-----------------------|-----------------------|--------------|----------------|
|     | C54-TiSi <sub>2</sub> | C54-TiGe <sub>2</sub> | Experimental |                |
| 311 | 2.297                 | 2.397                 | 2.311        | 0.137          |
| 004 | 2.135                 | 2.216                 | 2.145        | 0.124          |
| 022 | 2.087                 | 2.187                 | 2.100        | 0.130          |
| 313 | 1.828                 | 1.904                 | 1.836        | 0.101          |

corresponding experimental values estimated from Fig. 1(b). Representing the composition of this solid solution as Ti(Si<sub>1-y</sub>Ge<sub>y</sub>)<sub>2</sub>, the average Ge fraction, y, can be evaluated to be 0.12 from this result. Thus it can be concluded that Ti(Si<sub>1-y</sub>Ge<sub>y</sub>)<sub>2</sub> with a Ge fraction of y=0.12 is formed at the Ti/Si<sub>0.8</sub>Ge<sub>0.2</sub> interface due to annealing at 650 °C. This fact also suggests that Ge atoms are swept up into the SiGe layer at the interface. The production of Ge-rich Si<sub>1-x</sub>Ge<sub>x</sub> layers at the interface is thought to be likely, since the heat of formation in TiSi<sub>2</sub> and TiGe<sub>2</sub> is -57.0 and -47.5 kJ/mol,<sup>16</sup> respectively,

In order to clarify the interfacial reaction between Ti and Si<sub>1-x</sub>Ge<sub>x</sub>, XPS measurements were performed using 3.5-nm-thick Ti/Si<sub>0.5</sub>Ge<sub>0.5</sub>/Si(100) samples. Figure 2 shows XPS spectra of (a) Si 2p and (b) Ge 2p on Ti/Si<sub>0.5</sub>Ge<sub>0.5</sub>/Si(100) samples annealed at various temperatures. Although the

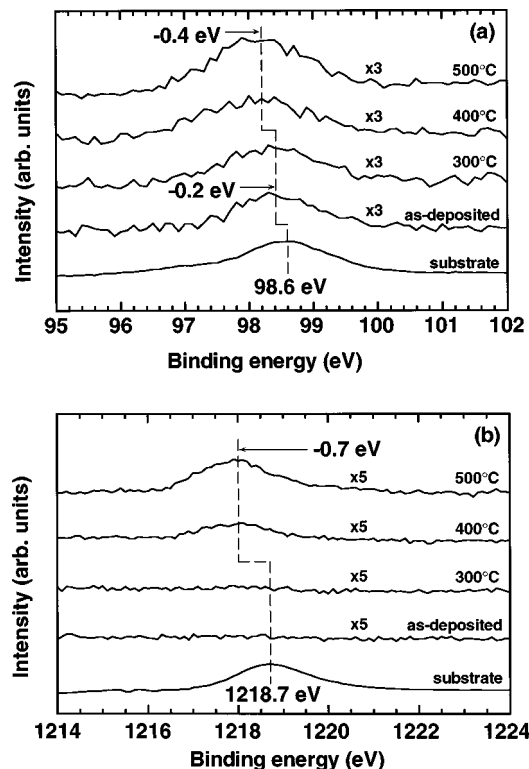


FIG. 2. XPS spectra of (a) Si 2p and (b) Ge 2p peaks of 3.5-nm-thick Ti/Si<sub>0.5</sub>Ge<sub>0.5</sub>/Si(100) before and after annealing at temperatures from 300 to 500 °C.

TABLE II. Measured binding energy shifts of XPS peaks in Ti/Si<sub>0.5</sub>Ge<sub>0.5</sub>/Si(100) and Ti/Ge(100) systems.

| Peak                                   | As-deposited | 300 °C         | 400 °C         | 500 °C  |
|----------------------------------------|--------------|----------------|----------------|---------|
| Ti/Si <sub>0.5</sub> Ge <sub>0.5</sub> | Si 2p        | -0.2 eV        | -0.2 eV        | -0.4 eV |
|                                        | Ge 2p        | N <sup>a</sup> | N <sup>a</sup> | -0.7    |
|                                        | Ti 2p        | 0              | +0.2           | +1.0    |
| Ti/Ge(100)                             | Ge 2p        | N <sup>a</sup> | -0.9           | -0.7    |
|                                        | Ti 2p        | 0              | +0.6           | +1.1    |

<sup>a</sup>N: not observed.

Si 2p peak can be observed even for as-deposited samples, the Ge 2p peak appears above 400 °C. In as-deposited and 300 °C annealed samples, a chemical shift of Si 2p by -0.2 eV occurs from the binding energy for bulk Si. At 400 and 500 °C, the chemical shifts of Si 2p and Ge 2p are -0.4 and -0.7 eV from the energy position for bulk Si and Ge, respectively.

The behavior of the Ge 2p peak in Fig. 2(b) is similar to that in the case of Ti/Ge(100) systems. The chemical shifts of XPS peaks in Ti/Ge(100) systems for various annealing temperatures are summarized in Table II, together with the results of Ti/Si<sub>0.5</sub>Ge<sub>0.5</sub>/Si(100). The Ge 2p signal is not observed below 300 °C, which is the same as the case of Ti/Si<sub>0.5</sub>Ge<sub>0.5</sub>/Si. The Ge 2p peak appears at a binding energy lower by -0.9 eV than the bulk Ge peak after annealing at 400 °C and the chemical shift is -0.7 eV at 500 °C. The Ti 2p peak shifts toward the higher binding energy with an increase in annealing temperature and the chemical shift is very close to that in Ti/Si<sub>0.5</sub>Ge<sub>0.5</sub>/Si. In the case of Ti/Si(100) systems, on the other hand, the silicidation causes the Si 2p and Ti 2p peaks to shift by -0.4 and +0.3 eV from bulk Si and metallic Ti,<sup>17,18</sup> respectively. Therefore, the relatively large chemical shifts of Ge 2p and Ti 2p are considered to be due to the bonding between Ti and Ge atoms. These results clearly indicate that Ti atoms preferentially react with Si atoms below 300 °C and the reaction with Ge atoms starts above 400 °C. This finding is consistent with the results of XRD measurements as mentioned above.

The depth profiles of Ti, Si, and Ge atoms measured by AES are shown in Fig. 3 for 50-nm-thick Ti/Si<sub>0.8</sub>Ge<sub>0.2</sub>/Si(100) annealed at 400 °C. It is noted that the composition ratio of Ge and Si atoms increases at the Ti/Si<sub>0.8</sub>Ge<sub>0.2</sub> interface. This result also supports the fact that the Ge-rich Si<sub>1-x</sub>Ge<sub>x</sub> layer is formed by the reactivity difference between Si and Ge atoms with Ti atoms at the interface.

## B. Electrical characteristics

The Schottky barrier heights of Ti/Si<sub>0.8</sub>Ge<sub>0.2</sub>/Si(100) and Ti/Si(100) diodes are shown in Fig. 4 as a function of annealing temperature. The Schottky barrier heights of Ti/n-Si<sub>0.8</sub>Ge<sub>0.2</sub> diodes are almost identical to those of Ti/n-Si(100) below 300 °C and decrease by annealing above 450 °C. In the case of Ti/p-Si<sub>0.8</sub>Ge<sub>0.2</sub> diodes, on the other hand, the Schottky barrier heights lower than that of

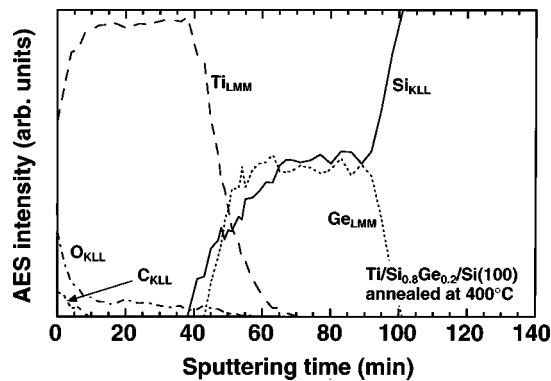


FIG. 3. AES depth profiles of Ti, Si and Ge atoms for 5.0-nm-thick Ti/Si<sub>0.8</sub>Ge<sub>0.2</sub>/Si(100) annealed at 400 °C.

Ti/*p*-Si(100) are obtained at temperatures below 300 °C and then the values are increased above 450 °C. In the case of pseudomorphic *p*-Si<sub>0.8</sub>Ge<sub>0.2</sub> layers used in this experiment, the Schottky barrier height can be expected to be lower by about 0.1 eV than that for metal/*p*-Si, since the band gap  $E_g$  is about 1.0 eV for a Ge fraction of  $x = 0.2$ .<sup>10</sup> The lowering of Schottky barrier heights at temperatures below 300 °C is more than the expected value of about 0.1 eV. The sum of the Schottky barrier heights of *n*- and *p*-type diodes,  $q(\phi_{Bn} + \phi_{Bp})$ , is shown in Fig. 5. The sum of Schottky barrier heights for Ti/Si(100) has an almost constant value below 600 °C although the value is slightly lower than the band gap of Si. In the case of Ti/Si<sub>0.8</sub>Ge<sub>0.2</sub> the sum is about 0.9 eV and gradually decreases with increasing annealing temperature.

As mentioned above, Ti atoms preferentially react with Si atoms and a Ge-rich layer tends to form at Ti/Si<sub>1-x</sub>Ge<sub>x</sub> interfaces as a result of solid-phase reaction. The Ge fraction

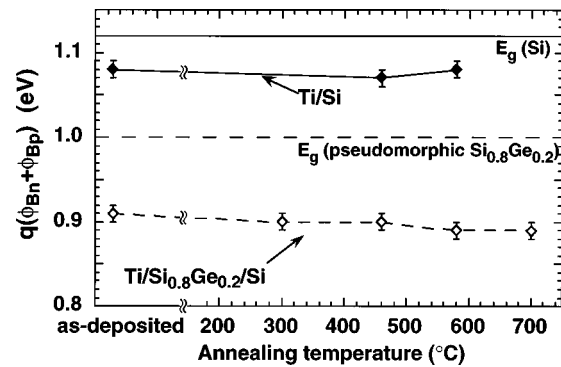


FIG. 5. Sum of Schottky barrier heights of *n*- and *p*-type diodes obtained in Fig. 7, as a function of annealing temperature. The energy band gap of Si and pseudomorphic Si<sub>0.8</sub>Ge<sub>0.2</sub> are also indicated.

of Ge-rich layers estimated from AES measurements is 0.3–0.4 for as-deposited and 400 °C-annealed samples. The measured values of  $q(\phi_{Bn} + \phi_{Bp})$  are relatively close to the band gap of Si<sub>1-x</sub>Ge<sub>x</sub> with  $x = 0.3$ –0.4,  $E_g = 0.9$ –0.85 eV. These facts suggest that the Schottky barrier height is affected by the chemical composition of Ge-rich layers formed at the interface. The other possible reason for the measured low barrier heights and low value of  $q(\phi_{Bn} + \phi_{Bp})$  for Ti/*p*-Si<sub>0.8</sub>Ge<sub>0.2</sub> annealed below 300 °C is an influence of defects existing at the interface. Indeed, the ideality factors of Ti/*p*-Si<sub>0.8</sub>Ge<sub>0.2</sub> diodes below 300 °C are about 1.3. However, after annealing at temperatures above 400 °C, the ideality factors are improved to below 1.2. For Ti/*n*-Si<sub>0.8</sub>Ge<sub>0.2</sub> diodes, the ideality factors are about 1.1 or less in this annealing temperature range. Therefore, the defects would partly contribute to the lowering of Schottky barrier heights in Ti/*p*-Si<sub>0.8</sub>Ge<sub>0.2</sub> below 300 °C.

It should be noted in Fig. 4 that the Schottky barrier heights for both *n*- and *p*-Si<sub>0.8</sub>Ge<sub>0.2</sub> are lower than those for *n*- and *p*-Si at annealing temperatures above 460 °C, respectively. At temperatures above 400 °C Ge atoms start to react with Ti atoms, and the Si<sub>0.8</sub>Ge<sub>0.2</sub> layer is strain relaxed above 460 °C, which is confirmed by XRD. Since the strain relaxation brings about an increase in the band gap and electron affinity of Si<sub>0.8</sub>Ge<sub>0.2</sub> layers,<sup>10</sup> it can be expected that the Schottky barrier heights for unstrained *n*- and *p*-Si<sub>0.8</sub>Ge<sub>0.2</sub> become low and high as compared with the strained case, respectively. The experimental results in Fig. 4 seem to be consistent with the change in band gap and electron affinity due to the strain relaxation. However, the values of  $q(\phi_{Bn} + \phi_{Bp})$  remain almost unchanged by annealing at temperatures above 460 °C. Therefore, the Schottky barrier heights at temperatures above 460 °C are thought to be mainly affected by the interfacial Ge-rich layer and the reaction product such as C54-Ti(Si<sub>1-y</sub>Ge<sub>y</sub>)<sub>2</sub>. From the application viewpoint, we can conclude that the Si<sub>1-x</sub>Ge<sub>x</sub>/Si structure is a favorable candidate for both *n*<sup>+</sup>- and *p*<sup>+</sup>-Si in achieving low-resistivity contacts.

The measured and calculated contact resistivities for *n*<sup>+</sup>- and *p*<sup>+</sup>-Si<sub>0.8</sub>Ge<sub>0.2</sub> are shown in Fig. 6 as a function of doping concentration. The solid and dashed lines are calculated

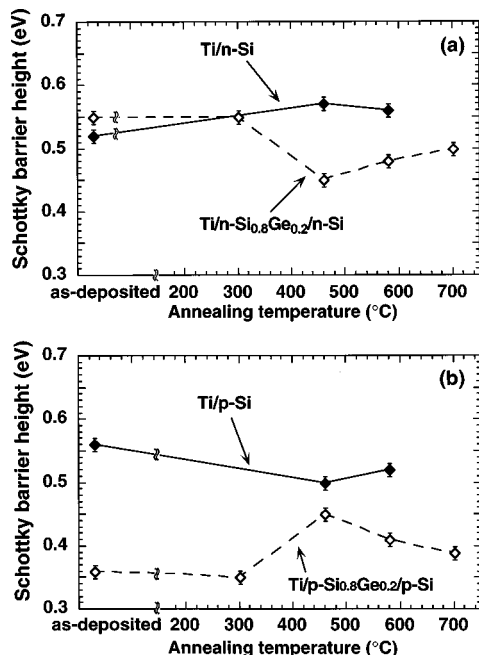


FIG. 4. Schottky barrier heights of Ti/Si<sub>0.8</sub>Ge<sub>0.2</sub>/Si(100) and Ti/Si(100) diodes for (a) *n*- and (b) *p*-type, as a function of annealing temperature.

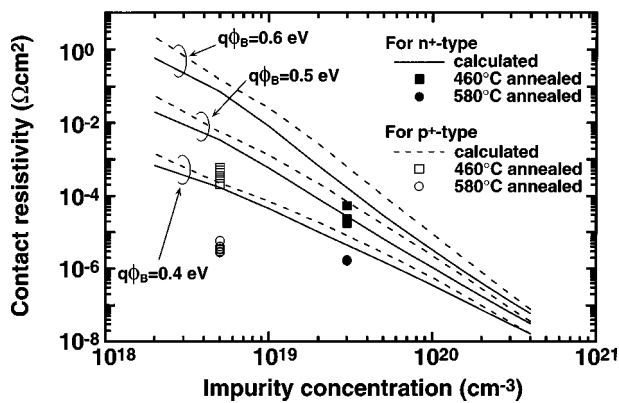


FIG. 6. Dependence of contact resistivities on substrate doping concentration for  $\text{Ti/Si}_{0.8}\text{Ge}_{0.2}/\text{Si}(100)$ . Solid and dashed lines are the calculated results based on the impurity band model proposed by Baltensperger (see Ref. 19).

curves for  $n^+$ - and  $p^+$ -type contacts, respectively.<sup>8</sup> In this calculation, a simple impurity band model proposed by Baltensperger<sup>19</sup> has been used, in which hydrogenlike centers with a regular impurity distribution and a Gaussian-type density-of-states function are assumed. In addition, both the thermionic emission and tunneling processes are also included as the transport mechanisms.<sup>20</sup> Since the effect of impurity bands is small at the doping concentrations below  $5 \times 10^{19} \text{ cm}^{-3}$ , we can expect that the experimental results are in good agreement with the calculated ones. The measured contact resistivities of  $\text{Ti/Si}_{0.8}\text{Ge}_{0.2}/\text{Si}(100)$  annealed at  $460^\circ\text{C}$  are very close to the calculated values for the Schottky barrier height of  $n$ - and  $p$ - $\text{Si}_{0.8}\text{Ge}_{0.2}$ . In the  $580^\circ\text{C}$  annealed case, however, the contact resistivities for  $n^+$ - and  $p^+$ - $\text{Si}_{0.8}\text{Ge}_{0.2}$  are 1/10–1/100 times as low as the values expected from the Schottky barrier heights. The contact resistivity is not only ruled by the Schottky barrier height but also by the doping concentration in Si substrates. For Ti/Si systems, it has been reported that the grain boundary diffusion of Ga and Sb atoms in  $\text{TiSi}_2$  is slow below  $600^\circ\text{C}$ .<sup>21</sup> Since the interfacial reaction proceeds at temperatures below  $600^\circ\text{C}$ , the dopant atoms would accumulate at the interface if the diffusion of dopant atoms into  $\text{Ti}(\text{Si}_{1-y}\text{Ge}_y)_x$  layers were sufficiently slow. Thus, one of the possible explanations for the decrease in contact resistivity at  $580^\circ\text{C}$  is the segregation of dopant atoms at the interface. Defects at the interface are also considered to be responsible for lowering the contact resistivity. Further investigation is necessary to clarify the behavior of dopant atoms and defects.

The other important factor to be considered for an application in the case of ULSI contacts is the relationship between the sheet resistance and the crystallographic structure. In the case of  $\text{TiSi}_2$ , it is known that the high-temperature phase of C54- $\text{TiSi}_2$  has a sheet resistance much lower than the low-temperature phase of C49- $\text{TiSi}_2$ .<sup>22</sup> Figure 7 shows the sheet resistance of 50-nm-thick  $\text{Ti/Si}_{0.8}\text{Ge}_{0.2}/\text{Si}(100)$ ,  $\text{Ti/Si}(100)$  and  $\text{Ti/Ge}(100)$  systems, as a function of annealing temperature. The sheet resistance of Ti/Si decreases by annealing at temperature above  $400^\circ\text{C}$  and has a minimum value of  $1.2 \text{ } \Omega/\square$  above  $550^\circ\text{C}$ , which is almost the

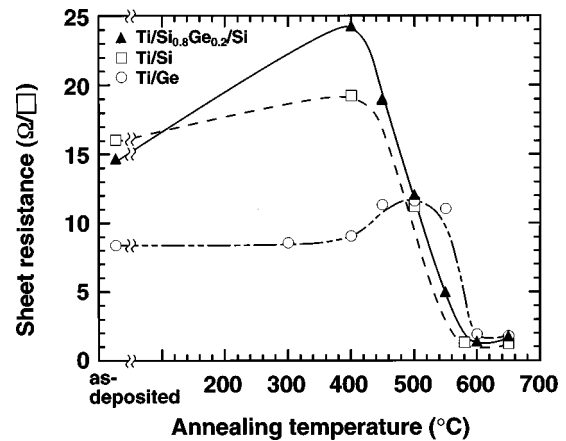


FIG. 7. Sheet resistance of 50-nm-thick  $\text{Ti/Si}_{0.8}\text{Ge}_{0.2}/\text{Si}(100)$ ,  $\text{Ti/Si}(100)$  and  $\text{Ti/Ge}(100)$ , as a function of annealing temperature.

same as a previously reported value.<sup>23</sup> In the case of  $\text{Ti/Si}_{0.8}\text{Ge}_{0.2}/\text{Si}$ , the sheet resistance has a maximum value of  $24.3 \text{ } \Omega/\square$  at  $400^\circ\text{C}$  and a minimum value of  $1.4 \text{ } \Omega/\square$  is obtained at  $600^\circ\text{C}$ . Above  $600^\circ\text{C}$ ,  $\text{Ti}(\text{Si}_{1-y}\text{Ge}_y)_2$  is formed as the reaction product in  $\text{Ti/Si}_{0.8}\text{Ge}_{0.2}/\text{Si}$  systems, as shown in Fig. 1(b). This fact indicates that C54- $\text{TiGe}_2$  is also a low-resistivity phase in addition to C54- $\text{TiSi}_2$ . Indeed, the Ti/Ge system exhibits the same annealing behavior of sheet resistance as the Ti/Si system, as seen in Fig. 7. The sheet resistance of Ti/Ge systems is about  $11 \text{ } \Omega/\square$  in the annealing temperature range of  $450$ – $550^\circ\text{C}$ , in which  $\text{Ti}_6\text{Ge}_5$  is formed, and decreases to  $1.8 \text{ } \Omega/\square$  by the formation of C54- $\text{TiGe}_2$  above  $600^\circ\text{C}$ .

#### IV. CONCLUSIONS

The Schottky barrier heights, contact resistivities and solid-phase reaction at the interface of  $\text{Ti/Si}_{0.8}\text{Ge}_{0.2}/\text{Si}(100)$  systems have been investigated in the annealing temperature range from  $300$  to  $700^\circ\text{C}$ . Silicon atoms preferentially react with Ti atoms at annealing temperatures below  $300^\circ\text{C}$  and Ge atoms start to react above  $400^\circ\text{C}$ . The low Schottky barrier heights are obtained for  $\text{Ti}/p\text{-Si}_{0.8}\text{Ge}_{0.2}$  below  $300^\circ\text{C}$ , whose values are smaller than those expected from the Ge reaction. For both  $n$ - and  $p$ -type diodes, the Schottky barrier heights lower than those of Ti/Si are obtained at annealing temperatures above  $460^\circ\text{C}$ . The sum of the Schottky barrier heights of  $n$ - and  $p$ - $\text{Ti/Si}_{0.8}\text{Ge}_{0.2}$  is smaller than the band gap of  $\text{Si}_{0.8}\text{Ge}_{0.2}$  in the whole temperature range. Furthermore, C54- $\text{TiSi}_2$  and C54- $\text{TiGe}_2$  are completely miscible and the formation of C54- $\text{Ti}(\text{Si}_{1-y}\text{Ge}_y)_2$  with a fraction of  $y = 0.12$  can be confirmed at  $650^\circ\text{C}$ . These results indicate that the Ge fraction is considered to be increased at the interface. The contact resistivities for  $n^+$ - and  $p^+$ - $\text{Si}_{0.8}\text{Ge}_{0.2}$  are close to the values expected from the Schottky barrier heights at  $460^\circ\text{C}$ ; however, the much lower values are obtained at  $580^\circ\text{C}$ . It is concluded that the SiGe interlayer can be expected upon realizing low resistivity contacts. C54- $\text{Ti}(\text{Si}_{1-y}\text{Ge}_y)_2$  and C54- $\text{TiGe}_2$  have sheet resistances as low as that of C54- $\text{TiSi}_2$ .

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