Properties of Schottky contact of Al on SiGe alloys

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(Received 25 April 1995; accepted for publication 17 December 1995)

Electrical properties of Schottky contacts of Al on p-$Si_{1-x}Ge_x$ alloys were investigated. The $Si_{1-x}Ge_x$ strained layers were grown on p-Si substrates by using rapid thermal process/very low pressure-chemical vapor deposition. Low reverse currents were obtained. It was found that the Schottky barrier height of Al/p-$Si_{1-x}Ge_x$ contacts decreased with increasing Ge fraction. The decrement is in accordance with the decrement of the band gap of the strained $Si_{1-x}Ge_x$. The Fermi level at the interface is pinned at about 0.43 eV below the conduction band. The influence of strain relaxation for SiGe alloy layers and the Si sacrificial cap layers on the properties of Schottky contacts were also investigated. © *1996 American Institute of Physics.* [S0003-6951(96)04508-2]

Metal/SiGe Schottky contacts are essential parts of some novel SiGe devices. The studies on this area are therefore very important. In recent years, interfacial reaction and properties of Schottky contacts for Pt, Pd, Ni, Ti, W–$Si_{1-x}Ge_x$ have been studied.[1–5] Pt/$Si_{1-x}Ge_x$ and Pd/$Si_{1-x}Ge_x$ Schottky contacts and their application in long-wavelength infrared detectors have been reported.[6,7] Schottky barrier height can be modulated by selecting Ge fraction, to obtain longer cutoff wavelength and increase the quantum efficiency of the detectors.[6,7] In older silicon technologies, metal aluminum is commonly used to form Schottky diodes due to its low cost, simple fabrication technology. However, Al and Si form an alloy, not a stable silicide like the above-mentioned metals.

In this work, Al/p-strained $Si_{1-x}Ge_x$ Schottky contacts were fabricated and their electrical properties were measured. The effect of the Ge fraction and the strain relaxation on Schottky barrier heights, and the influence of Si sacrificial cap layers on the properties of Schottky contacts were investigated.

$Si_{1-x}Ge_x$ alloy layers were epitaxially grown on p-type (100)Si substrates by computer controlled rapid thermal process/very low pressure-chemical vapor deposition (RTP/VLP-CVD).[8] Si buffer layers with a thickness of about 60 nm and p-$Si_{1-x}Ge_x$ alloy layers with boron doping concentration of about 1×10^{16} cm^{-3} were grown at 600 °C and a rate of 0.1–0.2 nm $^{-1}$. In order to investigate the effect of Ge fraction x and the thickness of $Si_{1-x}Ge_x$ layers on the properties of Schottky contacts, x values were selected to be 0, 0.17, 0.20, 0.25, and the thickness of SiGe ranged from 50 to 350 nm. Two sets of samples were fabricated with the same growth conditions to observe the influence of Ge segregation at the Al/SiGe interfaces. The first set had Si cap layers with a thickness of about 10 nm grown epitaxially on the $Si_{1-x}Ge_x$ layers, while the second set had no Si cap layers. The aluminum was vacuum evaporated and alloyed at a temperature of 430 °C. The area of the diode is 1.96×10^{-3} cm^{-2}.

The lattice parameter and strain of SiGe layers were measured by x-ray diffraction (XRD). The Ge fraction, boron doping concentration, and the thickness of the layers were determined by secondary ion mass spectroscopy (SIMS) and Auger electron spectroscopy (AES).

The electrical properties of Al/p-$Si_{1-x}Ge_x$ Schottky contacts were characterized by current–voltage (I–V) measurements. The I–V characteristics were analyzed with a thermionic emission model.[9] Schottky barrier height Φ_B and ideality factor n can be extracted from forward I–V curves.[9] The effective Richardson constant was estimated by using a linear dependence on the Ge composition.

Figure 1 shows the forward I–V characteristics of four Si layer capped Al/$Si_{1-x}Ge_x$ samples with $x=0$, 0.17, 0.20, and 0.25, respectively, and the reverse I–V characteristics of the sample with $x=0.20$ at room temperature. At 0.4 V reverse bias, the reverse current density is as low as 7.0×10^{-5} A cm^{-2}. The thickness of SiGe layers for the first three samples is 180 nm, while for sample No. 4, it is 120 nm. All of these are smaller than or near-critical thickness, and the SiGe layers are strained.[10] The barrier height Φ_B and ideality factor n calculated from the forward I–V curves are listed in Table I. The band-gap E_g of the $Si_{1-x}Ge_x$ strained layers,[10] the barrier height differences $\Delta\Phi_B$, the $Si_{1-x}Ge_x$ band-gap differences, ΔE_g, between two adjacent numbered samples and the differences $E_g-\Phi_B$ between band gaps and barrier heights are also listed in Table I.

It can be seen from Table I that the Schottky barrier height Φ_B decreases with increasing Ge fraction x and the decrements $\Delta\Phi_B$ are similar to ΔE_g. All the calculated differences between E_g and $q\Phi_B$ (position of barrier heights

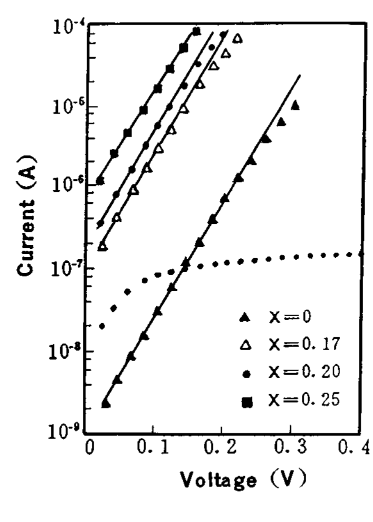

FIG. 1. I–V characteristics for Al/p-$Si_{1-x}Ge_x$ Schottky contacts ($x=0$, 0.17, 0.20, 0.25).

TABLE I. Φ_B, n, and E_g for Al/p-$Si_{1-x}Ge_x$ Schottky contacts with different Ge fractions. Among them, the E_g is quoted from Ref. 10, Φ_B, n and other values are estimated from the $I-V$ characteristics of the samples.

Sample No.	Ge fraction	n	Φ_B (V)	$\Delta\Phi_B$[a] (V)	E_g (eV)	ΔE_g[b] (eV)	$E_g - q\Phi_B$ (eV)
1	0	1.20	0.690		1.12		0.430
				0.099		0.10	
2	0.17	1.15	0.591		1.02		0.429
				0.016		0.02	
3	0.20	1.14	0.575		1.00		0.425
				0.035		0.04	
4	0.25	1.24	0.540		0.96		0.420

[a] $\Delta\Phi_B = \Phi_B(i+1) - \Phi_B(i)$.
[b] $\Delta E_g = E_g(i+1) - E_{g1}$, where i represents the number of samples, $i = 1,2,3$.

relative to the conduction band) are about 0.43 eV, indicating that the Fermi levels at the Al/p-$Si_{1-x}Ge_x$ interfaces are pinned at about 0.43 eV below the conduction band.

Figure 2 is an energy band diagram for the Al/p-$Si_{1-x}Ge_x$ interface with Fermi level pinned relative to the conduction band. The band gap of strained $Si_{1-x}Ge_x$ decreases with increasing x ($x_2 > x_1$). The conduction band offset ΔE_c is neglected, because the band-gap offset ΔE_g mainly presents the valence band offset ΔE_v.[11]

Figure 3 shows Schottky barrier height and the band gap for strained $Si_{1-x}Ge_x$ as a function of the Ge fraction. The two curves are almost parallel, indicating that $\Delta\Phi_B$ and ΔE_g are almost the same and the Fermi level at interface is pinned relative to the conduction band.

In practical applications, thicker SiGe layers are often needed. But, when the SiGe layer are thicker than the critical thickness, they may be relaxed. In order to investigate the influence of strain relaxation on the properties of Schottky barrier, samples with Ge fraction of 0.2 and thickness of 50, 180, and 350 nm were fabricated. The reverse $I-V$ curve for 50 nm thick sample is almost linear and similar to that for Al/p-Si substrate. The reason is that the depletion region has crossed the 50 nm SiGe layer and reached to the Si substrate. For 180 nm thick (fully strained) and 350 nm thick (almost

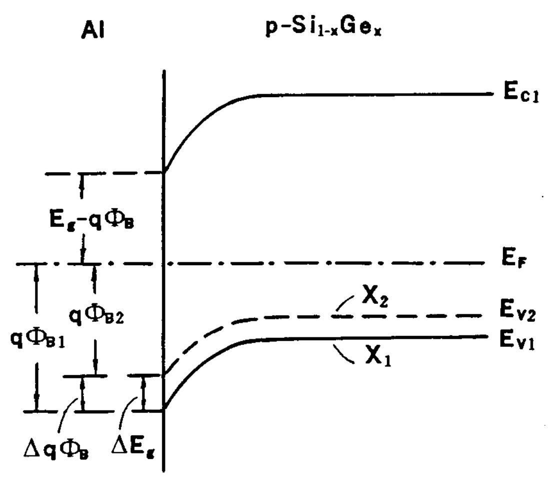

FIG. 2. Energy band diagram for Al/p-strained $Si_{1-x}Ge_x$ interfaces with Fermi level pinned relative to conduction band.

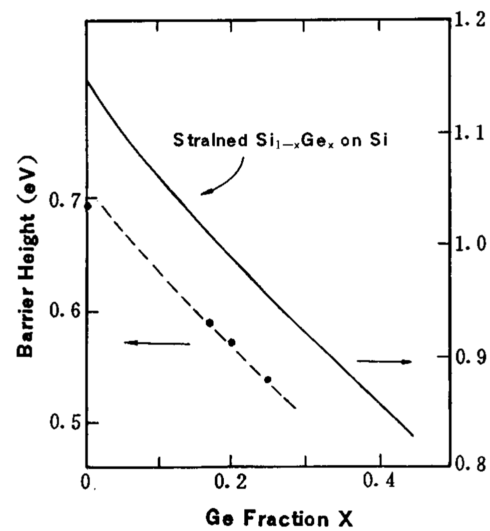

FIG. 3. Schottky barrier height and band gap for strained $Si_{1-x}Ge_x$ as a function of Ge fraction. The band gap is according to Ref. 10.

fully relaxed) samples, the $q\Phi_B$ values estimated from the forward $I-V$ curves were 0.575 and 0.63 eV, respectively. The difference is 0.055 eV, close to the 0.07 eV—difference between the band gaps of the above-mentioned two SiGe samples.[4,12] These results suggest that the barrier height increases with an increasing relaxation rate of SiGe strained layers. The Fermi level at the Al/p-relaxed $Si_{1-x}Ge_x$ interface is still pinned at about 0.43 eV below the conduction band.

Liou *et al.* investigated the interfacial reactions and Schottky barriers of Pt and Pd on epitaxial $Si_{1-x}Ge_x$ alloys, and found that during the Pt, Pd–$Si_{1-x}Ge_x$ reaction, Pt, Pd react preferentially with Si, resulting in Ge segregation and Fermi level pinning.[1] In order to investigate the possible Ge segregation for the direct contact between Al and SiGe, two sets of samples were prepared with and without Si cap layers on identical $Si_{0.8}Ge_{0.2}$ layers. Figure 4(a) is the Auger depth profile for a $Si_{0.8}Ge_{0.2}$ epitaxial layer with Si cap layer. Due to the Ge diffusion in the $Si_{0.8}Ge_{0.2}$ layer, the Si cap layer became a $Si_{1-y}Ge_y$ layer, and y decreased from $x=0.2$ at about 10 nm to $x=0.1$ at the surface. Figure 4(b) is the Auger depth profile of Al–$Si_{1-y}Ge_y$–$Si_{1-x}Ge_x$ after alloying. It shows that the Al alloys preferentially with Si. The Si in the cap layer is sacrificed to form the Al–Si alloy and the actual interface nearly reaches the $Si_{0.8}Ge_{0.2}$ layer. The $I-V$ characteristics of these two sets of samples indicate that the reverse current of the sample without the Si sacrificial cap layer is half an order of magnitude greater than that with a Si sacrificial cap layer (at 0.4 V reverse bias, the current density is 2.5×10^{-4} A cm^{-2}), and the barrier height $q\Phi_B$ increases from 0.575 to 0.60 eV. It can be inferred that when the $Si_{1-x}Ge_x$ (without the Si cap layer) reacts with Al, Si and Al preferentially react while the Ge segregates and results in defects at the interface.

In conclusion, Al/p-SiGe Schottky contacts have been grown successfully by RTP/VLP-CVD. Low reverse currents were obtained. It was shown that the Schottky barrier height of Al/p-$Si_{1-x}Ge_x$ can be controlled by Ge fraction x. The

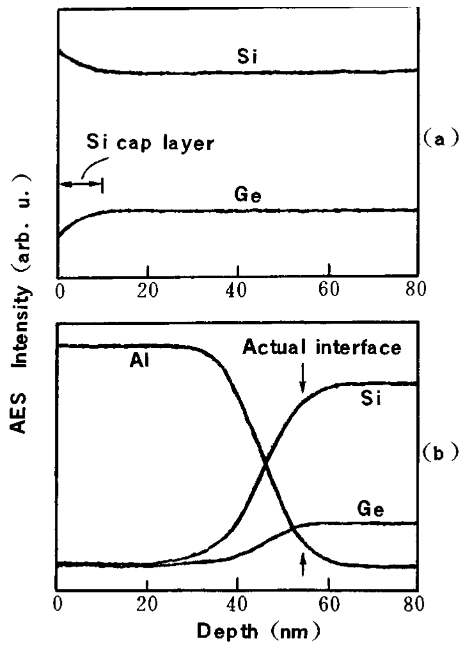

FIG. 4. Auger depth profile of (a) Si cap(10 nm)–$Si_{0.8}Ge_{0.2}$ structure and (b) Al–Si sacrificial cap–$Si_{0.8}Ge_{0.2}$ structure after alloying.

greater the Ge fraction, the lower the barrier height. The decrement of barrier height is in accordance with the decrement of the band gap of $Si_{1-x}Ge_x$ strained layer. The Fermi level at interface of Al/p-$Si_{1-x}Ge_x$ is pinned at about 0.43 eV below the conduction band.

When the thickness of the SiGe alloy layer is greater than critical thickness, strain relaxation occurs and the Schottky barrier height increases. The increment is basically similar to the increment of the band gap caused by strain relaxation. This indicates that the Fermi level of the relaxed SiGe layer is still pinned at about 0.43 eV below the conduction band.

The Si sacrificial cap layer is essential. It provides the Si for alloying preferentially with Al. With this layer, the Ge segregation at the interface can be minimized, and the increment of reverse current and barrier height will be avoided.

The authors gratefully acknowledge the 301 Group of Nanjing Electronic Devices Institute for their $I-V$ measurements.

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