12-9-1996

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Recommended Citation

J. Mi, A. Gupta, C.Y. Yang, J. Zhu, P.K.L. Yu, P. Warren, and M. Dutoit, "Properties of Schottky Contacts of Aluminum on Strained $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ Layers," *Applied Physics Letters* 69, 3743-3745 (1996). <https://doi.org/10.1063/1.117208>

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Properties of Schottky contacts of aluminum on strained $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ layers

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(Received 22 July 1996; accepted for publication 17 September 1996)

Schottky contacts of $\text{Al}/\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ were fabricated using conventional Si technology. Effects of thermal processing of the alloys on the electrical properties of the $\text{Al}/\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ Schottky diodes were investigated. Current-voltage (I - V), capacitance-voltage (C - V), and x-ray diffraction measurements were performed. These thick alloy films (100–150 nm) experienced strain relaxation upon annealing at 700 °C. Nearly ideal I - V and C - V behaviors were obtained for strain-compensated samples. I - V and C - V characteristics show evidence of dislocation-related traps for strain-relaxed samples. Carbon incorporation improves the I - V and C - V characteristics by lessening the extent of lattice relaxation due to thermal processing. © 1996 American Institute of Physics. [S0003-6951(96)03148-8]

Recently, $\text{Al}/\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y/\text{Si}$ heterostructures have attracted increased interest in Si-based technology,¹ since, compared with the binary alloy $\text{Si}_{1-x}\text{Ge}_x$, $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ can provide more flexible band-gap engineering, which enables silicon to compete with compound semiconductors in high-performance electronic and optoelectronic devices. Substitutional incorporation of carbon reduces the lattice strain introduced by germanium, and results in increased critical thickness of the alloy layers and separate control strain and composition. The major issues related to device applications include optimizing the heteroepitaxial growth, understanding the alloy electronic properties, and assessing the thermal stability of the alloy layers.

Defect-free $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y/\text{Si}$ heterostructures have been produced using rapid thermal chemical vapor deposition (RTCVD), and a process window for this technique compatible with silicon technology has been developed to growth high-quality SiGeC layers.^{2,3} It has been shown that as lattice strain was reduced through the addition of carbon, the band gap increased only slightly, alleviating the concern of band-gap reversion due to carbon incorporation.⁴ Even if the as-grown alloy layers are defect-free, there is still an important issue of stability when the alloy layers are subjected to subsequent thermal processing. Since there exists the possibility of silicon carbide precipitation, SiGeC layers are chemically metastable in addition to the inherent mechanical metastability of SiGe layers. Previous studies of thermal stability have focused on changes in lattice relaxation and carbide precipitation under *ex situ* stress (high-temperature annealing).^{5–8} Generally, as annealing temperature increases, lattice relaxation occurs. Silicon carbide precipitation, if present, would require higher temperature (above 950 °C).^{5,6,8} Studies of the effect of thermal processing on electrical properties of the

SiGeC/Si system have not been reported to date. In this letter, we report results of electrical measurements on Al/SiGeC Schottky diodes that were fabricated using conventional silicon processing. Unlike previous work, our investigation is focused on the effects of carbon incorporation on the electrical properties of the SiGeC alloy, using these Schottky diodes as test vehicles.

The alloy layers used to fabricate Al/SiGeC Schottky diodes were grown using RTCVD. The growth process is described in Ref. 2. Briefly, on *n*-type Si (100) substrates with phosphorus concentration of about $5 \times 10^{15} \text{ cm}^{-3}$, an undoped Si epilayer of 200 nm was grown as a buffer layer followed by an undoped alloy layer of 100–150 nm depending on the composition. $\text{Si}_{1-x}\text{Ge}_x$ layers were obtained with compressive strain of 1.5% ($x=0.2$). The carbon concentration in $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ layers varies from 0 to 2 at. %. Analyses of the alloy layers show that they are free of structural defects and precipitation of silicon carbide, and all carbon atoms are in substitutional sites.³ Using the hot-point-probe method, the alloy layer was determined to be *n* type. The dopant concentrations in the buffer and alloy layers are assumed to be about the same as that of the substrate because of dopant out diffusion during deposition. Two batches of Schottky diodes were fabricated (see Fig. 1). For the first

FIG. 1. Cross-sectional schematics of Schottky diodes used in this study: (a) with and (b) without donor implantation to form n^+ region for Al/alloy Ohmic contact.

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FIG. 2. I - V characteristics of Al/alloy Schottky diodes made with donor implantation and thermal activation.

batch [Fig. 1(a)], using a photoresist layer with a thickness of about $1\ \mu\text{m}$ as a mask, phosphorus was implanted into the alloy layer to ensure good electrical contact. The energy and dose of the implantation were $40\ \text{keV}$ and $5 \times 10^{13}\ \text{cm}^{-2}$, respectively. Donor activation was achieved with a furnace anneal in N_2 ambient at $700\ ^\circ\text{C}$ for 60 min. The second batch [Fig. 1(b)] was produced without phosphorus implantation but with one sample annealed using the same condition as for the first batch. Aluminum electrodes with areas of $2.8 \times 10^{-3}\ \text{cm}^2$ were formed using sputtering and standard wet patterning. While the implanted n^+ region substantially reduces the contact resistance at high biases ($>0.3\ \text{V}$), it does not have much effect on results at low biases. The two different batches allowed us to isolate the effects of thermal annealing. Capacitance-voltage (C - V) and current-voltage (I - V) measurements were performed at room temperature. X-ray diffraction (XRD) was used to measure alloy thickness and to monitor lattice relaxation.

I - V characteristics of the first batch of samples are shown in Fig. 2. Our focus is on the $\log I$ versus V behavior below $0.2\ \text{V}$. For the control Si epilayer, a straight line and an ideality factor $n=1.04$ are observed, indicating that the current is mainly due to thermionic emission and diffusion.⁹ However, the current and ideality factor of the SiGe sample are much higher than those of the Si epilayer, inferring that mechanisms other than thermionic emission and diffusion also contribute to the total current. On the other hand, both current and ideality factor decrease with increasing carbon concentration. For the sample with $y=0.02$, both parameters as well as the entire I - V curve are quite close to those for the Si epilayer.

C - V characteristics of the first batch of samples are shown in Fig. 3. In Fig. 3(a), a straight line is observed for the Si epilayer under reverse bias, indicating a uniform dopant concentration. For the SiGe sample, however, the $1/C^2$ - V curve is quite different. Figure 3(b) is an enlarged version of Fig. 3(a) so that the change in slope under reverse

FIG. 3. (a) C - V characteristics of Al/alloy Schottky diodes formed by donor implantation and thermal activation. (b) Enlargement of (a).

bias is more apparent. There are two slopes for each of the SiGe and SiGeC curves, a smaller one at low biases, which increases with increasing carbon concentration, and a larger one at high biases, which is essentially the same for all samples.

As a first approximation, we assume that in the low-bias range, the depletion width W and dopant concentration N_D of the samples can be calculated from the capacitance and the slope of the $1/C^2$ versus V curve, respectively,⁹ although the annealed samples are expected to be defective, which might give rise to significant leakage current in the reverse-biased regime. However, we have determined the reverse-biased currents for the annealed samples to be less than $6\ \text{nA}$ at $-5\ \text{V}$. Table I presents the values of the parameters obtained from XRD and C - V measurements for the first batch of samples. t_{alloy} (XRD) is the thickness of the as-grown alloy layer measured by XRD. W' is the reverse-biased depletion width calculated from the capacitance at which the $1/C^2$ versus V slope varies most rapidly. W_0 is the zero-biased depletion width. The values of t_{alloy} (XRD) and W' are in good agreement for sample A, justifying the above assumption. For samples B and C, the values of W' are meaningless if used to compare with those of t_{alloy} (XRD), since W_0 is already larger than t_{alloy} (XRD) for these samples. A dopant concentration of $7.9 \times 10^{15}\ \text{cm}^{-3}$ for the Si sample is reasonably close to the approximate substrate dopant of $5 \times 10^{15}\ \text{cm}^{-3}$. It is also seen that the doping in SiGe is much higher than that in the Si epilayer.

Figure 4 shows the $1/C^2$ versus V curves for the second

TABLE I. Parameters of $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ layers extracted from XRD and C - V measurements.

Sample	x	y	t_{alloy} (XRD) (nm)	W' (CV) (nm)	W_0 (CV) (nm)	N_D (cm^{-3})
Si	0	0	...	...	420	7.9×10^{15}
A	0.2	0	150	145	65	1.9×10^{17}
B	0.2	0.016	135	...	140	4.4×10^{16}
C	0.2	0.020	105	...	270	1.6×10^{16}

FIG. 4. C - V characteristics of Al/alloy Schottky diodes without donor implantation. A SiGe sample was annealed as in the first batch.

batch of Schottky diodes with one SiGe sample annealed under the same condition as that used for the first batch. As expected, the slopes for the unannealed samples are approximately the same. In addition, for the annealed SiGe sample, behavior similar to its counterpart in the first batch is observed. Thus, thermal annealing leads to defect formation that degrades the C - V characteristics.

It is known that carbon incorporation improves the structural stability of SiGe alloys deposited on Si.⁸ Without strain compensation by carbon, strained SiGe layers may relax due to thermal annealing. This effect is demonstrated for the $\text{Si}_{0.8}\text{Ge}_{0.2}$ sample with a thickness (150 nm) much larger than the equilibrium critical thickness of about 20 nm for this germanium concentration.¹⁰ [004] XRD rocking curves for this sample before and after annealing are shown in Fig. 5. The positive shift of the alloy peak towards the substrate peak (normalized at 0°) is an indication of the decrease of the out-of-plane lattice constant due to annealing. From the shift, one can estimate that 85% of the lattice strain, defined as the ratio of the out-of-plane lattice constant of the alloy layer to that of the Si substrate, relaxed after thermal annealing.

The above results show that carbon incorporation improves the I - V and C - V characteristics of Al/alloy contacts. It is known that dislocations form in thick SiGe films that have been annealed,¹¹ and these dislocations are associated with traps.¹² Dislocation-related traps in SiGe were shown to degrade I - V characteristics of SiGe/Si heterojunctions through an increase in recombination current.¹³ On the other hand, our C - V measurements imply that there are additional electrically active defects in the *annealed* alloys layers. Donor complexes formed via strain relaxation in SiGe layers were previously observed.¹⁴ Recombination via traps and tunneling due to high doping can occur in carrier trans-

FIG. 5. [004] XRD rocking curves of a $\text{Si}_{0.8}\text{Ge}_{0.2}$ sample before and after thermal annealing.

port across Schottky contacts.⁹ It is likely in our degraded samples that the dislocations due to annealing introduce traps, which simultaneously act as recombination centers and manifest themselves as ionized donorlike impurities in capacitance measurements.

For a given annealing condition, the trap density depends on the degree of lattice relaxation. Since strain energy in the alloy layer decreases with increasing carbon concentration, nearly ideal I - V and C - V characteristics can be obtained for strain-compensated Al/SiGeC Schottky diodes. Chemical relaxation due to silicon carbide precipitation is not likely for our samples since the anneal temperature used here is lower than that for the onset of carbide precipitation.⁵⁻⁸

In conclusion, the effects of thermal processing of the strained $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y/\text{Si}$ system on the electrical characteristics of Al/ $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ Schottky diodes have been investigated. I - V and C - V characteristics were obtained for $\text{Si}_{1-x}\text{Ge}_x$ with germanium content of 20 at. % and for $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ with carbon content up to 2 at. %. Dislocation-related traps were evident in the alloy layers for samples having been subjected to thermal processing. Our results provide evidence that the electrical properties of the ternary alloy SiGeC, unlike SiGe, can be engineered to resemble those of the corresponding Si underlayer.

The authors wish to thank K. Tan (Santa Clara University) for technical assistance, R. King (Stanford University) for aluminum sputtering, and M. Prisbe (Stanford University) for assistance with photolithography. This work has been partially supported under a Stanford Nanofabrication Facility User Grant within the National Nanofabrication Users Network.

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