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Effects of Thermal Stability of $Si_{1-x-y}Ge_xC_y$ Layers on Properties of Their Contacts with Aluminum

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The effects of thermal stability of $Si_{1-x-y}Ge_xC_y$ layers on the electrical properties of Al/$Si_{1-x-y}Ge_xC_y$ Schottky diodes have been investigated. I-V, C-V, and x-ray diffraction measurements were performed to examine the electrical properties and lattice structure of the alloy layers. Nearly ideal I-V and C-V characteristics were obtained for $Si_{1-x-y}Ge_xC_y$ with strain reduced substantially by carbon incorporation. High effective dopant concentration was observed for strained alloy layers, which had been subjected to thermal annealing. This effective doping is attributed to lattice-relaxation related defects.

1. Introduction

Recently, $Si_{1-x-y}Ge_xC_y$/Si heterostructures have attracted increased interest in Si-based technology[1], since, compared with the binary $Si_{1-x}Ge_x$ alloy, $Si_{1-x-y}Ge_xC_y$ alloy can provide more flexible bandgap engineering. Carbon incorporation reduces the strain induced by germanium in the alloy layers and thus improves their mechanical stability. In addition, the ternary alloy has an additional degree of freedom in bandgap design. One of the major issues related to device application is the thermal stability of SiGeC layers. Since there exists the possibility of silicon carbide precipitation, SiGeC layers are chemically metastable in addition to the inherent mechanical metastability that exists in SiGe layers. Previous studies of thermal stability have focused on physical and chemical changes of lattice structure such as relaxation and precipitation under *ex-situ* stress (high-temperature annealing)[2-4].

In this paper, we report results on electrical measurements of 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.

2. Experimental

The alloy layers used to fabricate Al/SiGeC Schottky diodes were grown by rapid thermal chemical vapor deposition. The growth process was described previously[5]. Briefly, on n-type (100)-Si substrates with phosphorus concentration of about $5x10^{15}$ cm^{-3}, an undoped Si epi-layer layer of 200 nm was grown as a buffer layer followed by an undoped alloy layer of 100 to 150 nm depending on the composition. $Si_{1-x}Ge_x$ layers were obtained with compressive strain up to 1.5% (x=0.2). The carbon concentration in $Si_{1-x-y}Ge_xC_y$ layers varies from 0 to 2 at%. Characterizations of the alloy layers show that they are free of structural defects and precipitation of silicon carbide. All the carbon atoms were confirmed to be in substitutional sites[6]. Two batches of Schottky diodes were fabricated. For the first batch, using a photoresist layer of about 1 μm as a mask, phosphorus was implanted into the alloy layer to ensure good electrical contact. The energy and dose of the implantation were 40 keV and $5x10^{13}$ cm^{-2}, respectively. Donor activation was achieved with a furnace anneal at 700 °C for 60 min in N_2. The second batch was produced without phosphorus implantation but with one sample annealed using the same condition of donor activation as for the first batch. Aluminum electrodes of $2.8x10^{-3}$ cm^2 were made by Al sputtering and wet patterning. While the n^+ zone under Al electrode did greatly enhance the rectifying characteristics at high biases (> 0.3 V), it did not have much influence on results at low biases. The two different processes allowed us to isolate the effects of thermal annealing. C-V and I-V measurements were performed at room temperature. X-ray diffraction (XRD) was used to monitor lattice relaxation.

3. Results and Discussion

Log (I) - V curves of the first batch of samples are shown in Fig. 1. From results in the low-bias regime, an ideality factor of 1.04 was extracted for the Si epi-layer (reference sample). This implies that the current was a result of thermionic emission and/or diffusion[7]. The current and ideality factor of the SiGe sample were much higher than those of the reference sample, inferring that other mechanisms than the thermionic emission and diffusion also contributed to the total current. However, both current and ideality factor decrease with increasing C concentration. For the sample with 2 at% C, both parameters as well as the entire I-V curve are quite close to those for the Si epi-layer.

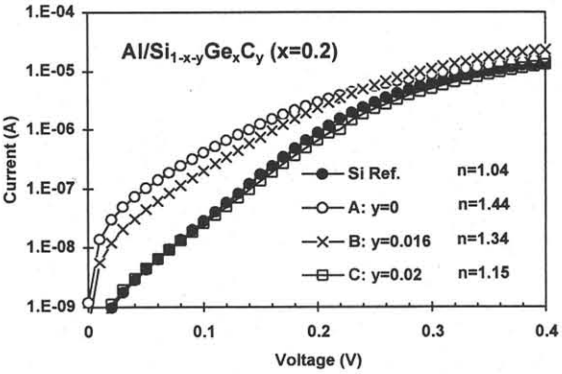

Fig. 1. I-V characteristics of Al/alloy Schottky diodes made with donor implantation and thermal activation.

$1/C^2$ - V curves from the first batch of samples are shown in Fig. 2. In the reverse-bias range, a straight line is observed for the Si epi-layer (Fig. 2a), with slope corresponding to doping concentration within the layer[7]. For the SiGe sample, however, the slope of $1/C^2$ - V curve is quite different from that of the Si epi-layer. Fig. 2b provides a closer look at the change of slope for each curve. It is clear that there are two slopes for each curve of SiGe and SiGeC samples at reversed bias, a smaller one at low bias, which increases with C concentration, and a larger one at high bias, which is essentially the same for all samples and corresponds to the epi-layer doping.

Table I summaries the parameters obtained from I-V and C-V measurements. t_{alloy}(XRD) is the thickness of the as-grown alloy layer measured by XRD. t_{alloy}(CV) is the depletion width calculated from the capacitance of $1/C^2$-V curve at which the slope varies most rapidly. The larger difference between t_{alloy}(XRD) and t_{alloy}(CV) for sample B and C is attributed to the change in slope occurring so close to zero bias that the capacitance is not due to depletion charge alone. From the values of N_D, which were calculated using low-bias slopes, it is seen that the doping concentration increases for the SiGe sample and decreases with increasing C concentration.

Fig. 3 shows $1/C^2$ - V curves for the second batch of Schottky diodes with one SiGe sample annealed under the same condition as used for the first batch. As expected, the slopes for the unannealed samples are approximately equal corresponding to the epi-layer doping. Behavior similar to that of the first batch is observed for the annealed sample, confirming that thermal annealing was the cause for high doping in the alloy layers.

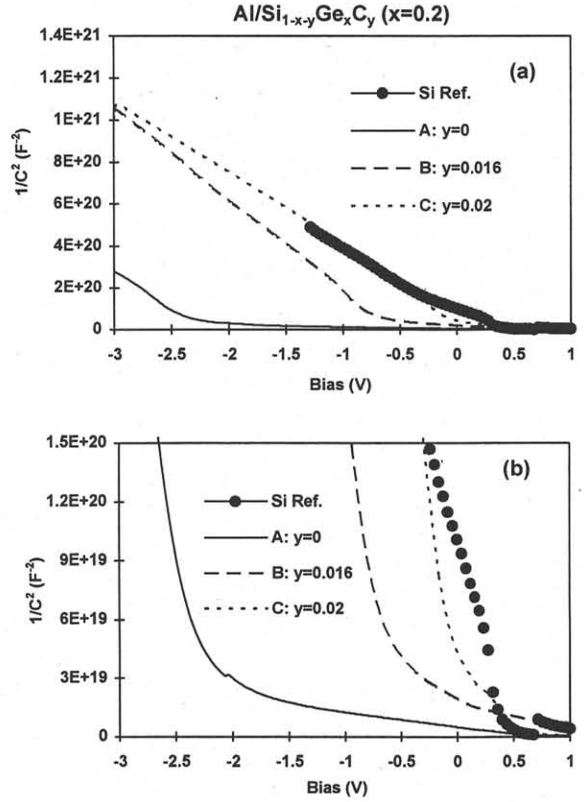

Fig. 2. (a): $1/C^2$-V curves from Al/alloy Schottky diodes formed by donor implantation and thermal activation. (b): Enlargement of (a).

Table I Parameters of $Si_{1-x-y}Ge_xC_y$ layers extracted from XRD and C-V measurements

	x	y	t_{alloy}(XRD) (nm)	t_{alloy}(CV) (nm)	N_D (cm^{-3})
Si	0	0	-	-	7.9E15
A	0.2	0	150	145	1.9E17
B	0.2	0.016	135	190	4.4E16
C	0.2	0.020	105	220	1.6E16

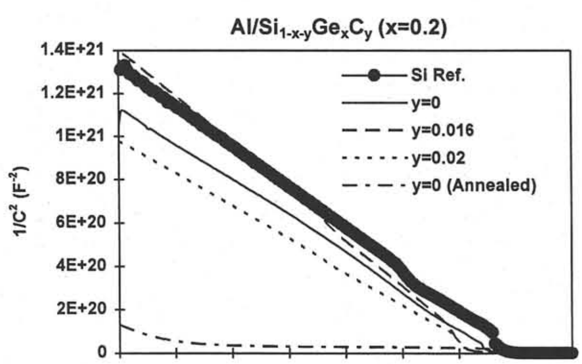

Fig. 3. $1/C^2$-V curves of Al/alloy Schottky diodes with one SiGe sample annealed.

It is known that C incorporation improves the structural stability of SiGe layers[4]. Without strain compensation by carbon, strained SiGe layers can relax due to thermal annealing. This was the case for the $Si_{0.8}Ge_{0.2}$ sample, since its thickness (150 nm) is much larger than the equilibrium critical thickness (about 20 nm) at this Ge concentration[8]. XRD rocking curves of this sample before and after annealing are shown in Fig. 4. The shift of the alloy peak towards the substrate peak is an indication of the decrease of out-of-plane lattice constant due to relaxation. From the shift, one can estimate that 85% of the lattice strain relaxed after thermal annealing.

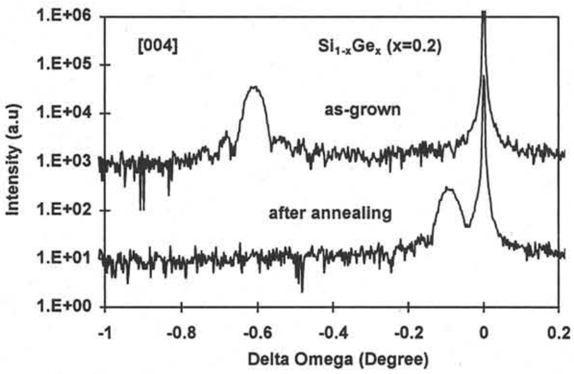

Fig. 4. [004] XRD rocking curves of the $Si_{0.8}Ge_{0.2}$ sample before and after thermal annealing.

The above results show that C incorporation improves the I-V and C-V characteristics of Al/alloy contacts. Since lattice relaxation introduces misfit dislocations, the final structure of the annealed alloy film could be very defective due to the presence of threading dislocations[9]. It is likely that the dislocations induce electrically active defects which in turn give rise to high doping found in the relaxed layers. Thus, electron tunneling due to high doping probably occurs during I-V measurements, resulting in higher current and larger ideality factor. The defect-related doping gives rise to an observed smaller slope in the $1/C^2$ - V curves as the depletion width expands from the alloy layer into the Si epi-layer. For a given annealing condition, the level of defect-related doping depends on the degree of lattice relaxation. Since strain energy in the alloy layer decreases with increasing C incorporation, nearly ideal I-V and C-V characteristics can be obtained for strain-compensated samples. 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[2-4].

4. Conclusion

The effects of thermal processing of strained SiGeC layer on the electrical properties of Al/SiGeC Schottky contacts have been investigated. I-V and C-V characteristics were obtained for $Si_{1-x}Ge_x$ with germanium content up to 20 at% and for $Si_{1-x-y}Ge_xC_y$ with carbon content up to 2 at%. Defect-related doping was evident from C-V characteristics in highly strained alloy layers subjected to thermal processing. This doping is attributed to defects induced by strain relaxation. Our results provide evidence that the electrical properties of SiGeC, unlike its binary counterpart SiGe, can be engineered to resemble those of the corresponding Si under-layer.

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