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Growth and Electrical Performance of Heterojunction p^+ $Si_{1-x-y}Ge_xC_y$/ p^- Si diodes

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Abstract

We have fabricated heterojunction p^+ $Si_{1-x-y}Ge_xC_y$/ p^- Si diodes. The SiGeC layers were grown epitaxially on Si (100) substrates by the rapid thermal chemical vapor deposition (RTCVD) technique using methysilane gas as a carbon precursor. The germanium concentration is 20% in these SiGeC alloys and the carbon concentrations are in the range of 0% to 1%. By studying the current-voltage characteristics of these diodes as a function of temperature the valence band discontinuities between SiGeC and Si layers were obtained as a function of carbon concentrations. We have found that the valence band discontinuity of the SiGe/Si heterostructure decreases by 11 meV when 1% of carbon is incorporated. Photoluminescence (PL) results show that 1% carbon increases the bandgap of strained p^+SiGe alloys by 25 meV. This would imply that the conduction band discontinuity of SiGe/Si will decrease by 14 meV when 1% carbon is incorporated.

Introduction

It is well known that strained SiGe layers grown on unstrained Si substrates have many device applications. Various device structures have been fabricated such as heterojunction bipolar transistors (HBT's) and different kinds of infrared (IR) detectors. However, due to the lattice mismatch between SiGe alloys and the Si substrates, the strain contained in the SiGe layers imposes a severe design constraint. There are limitations on the allowed thickness and/or Ge concentrations on the SiGe layers pseudomorphically grown on Si substrates before the generation of misfit dislocations.

In principle, it is possible to reduce the strain by incorporating carbon atoms substitutionally into the $Si_{1-x}Ge_x$ lattice to form $Si_{1-x-y}Ge_xC_y$ alloys due to the smaller size of carbon atom compared to that of Si and Ge. Indeed, it has been reported that the addition of small amounts of substitutional carbon reduce the level of strain. It has been found that 1% of carbon fraction can reduce the strain introduced by 8.3% of germanium [1]. Previous results also demonstrated that a carbon concentration as high as 2% can be introduced substitutionally into a $Si_{1-x}Ge_x$ layer by the low temperature non-equilibrium epitaxial technique[2], so that $Si_{0.82}Ge_{0.16}C_{0.02}$ layers would be essentially strain-free when grown on the (100) Si substrate.

In addition to reducing strain, PL has shown that the initial addition of carbon increases the bandgap of undoped pseudomorphic $Si_{1-x-y}Ge_xC_y$ alloys on Si (100) substrates. The bandgap increases by about 21-23 meV[3-4] when 1% of carbon is added. Given the bandgap increase, this will imply a change of valence and/or conduction band discontinuities of the SiGe/Si heterostructures when carbon is added into the SiGe layers. Since most of the long wavelength

infrared (LWIR) device applications of SiGe/Si heterostructures such as heterojunction internal photoemission (HIP's) [5] structures, PtSi/SiGe structures[6] and multiple quantum well (MQW) structures[7] are based on the valence band discontinuities, it is important to know the effect of carbon on the valence band discontinuity of the pseudomorphic $Si_{1-x-y}Ge_xC_y$ on Si (100) substrate.

In this paper, we report our results on the change of valence band discontinuities of $Si_{1-x-y}Ge_xC_y$ / Si as a function of carbon concentration. The results are based on the reverse biased current-voltage characteristics of p^+ $Si_{1-x-y}Ge_xC_y$/ p^- Si diodes as a function of temperature. We have also studied the effect of carbon on the bandgap of p^+ SiGeC alloys. Combining the effect of carbon on the bandgap of SiGeC and the valence band discontinuity of SiGeC/Si, we determine the conduction band discontinuity of $Si_{1-x-y}Ge_xC_y$ / Si.

Experimental details

SiGeC/Si heterostructures were grown by rapid thermal chemical vapor deposition (RTCVD). The growth temperature was 1000°C for Si and 625°C for SiGeC. Dichlorosilane (SiH_2Cl_2), germane (GeH_4) and methylsilane ($SiCH_6$) were use as the precursors of Si, Ge and C, respectively. The flow rates were 26 sccm for dichlorosilane, 1 sccm for germane, and 0 to 0.1 sccm for methylsilane. The chamber pressure was kept at 6 torr. Details of our growth system are available elsewhere[8].

The diode structures were grown on p^- Si (100) substrate and consisted of initial 1μm p^+ Si ($3x10^{19}/cm^3$) for a back contact and 2000A p^- ($10^{16}/cm^3$) Si layers, followed by a 25A undoped SiGeC spacer, 160A p^+ SiGeC($10^{19}/cm^3$) and final 240A p^{++} SiGe ($3x10^{19}/cm^3$) for a top contact. The SiGeC layers contain 20% Ge and various C concentrations ranging from 0% to 1% in the SiGeC layer. Diodes were fabricated by plasma etching to create a mesa followed by Al metallization. The p^+ SiGeC/ p^{++} SiGe interface was assumed to be electrically ohmic and not to affect the I-V curves. A schematic cross section of the device structure is shown in Fig(1). The mesa area is 320 x 180 μm^2 and the top contact area is 160 x 130 μm^2.

Another set of samples was grown for photoluminescence (PL) measurements. The structures are similar except that 38% [Ge] was used in the p+ SiGeC layer (for comparison with our previous PL results on the undoped SiGeC layer, containing 38% Ge) and that a 500 A p^+ Si layer was grown on top to form a single quantum well , instead of the p^{++} SiGe layer in the diodes.

Experimental results

Figure (2) shows the (400) x-ray diffraction (XRD) performed on the SiGeC layer containing 20% Ge and various C concentrations. The concentration of Ge was obtained by measuring the XRD peak relative to that of the Si substrate which gives us the vertical lattice constant of the strained SiGe epilayer. As more C was added , the peaks shift toward the Si peak, indicating decreased lattice constant, i.e., reduced strain. The C concentrations were determined by the shifts of XRD peaks using the Ge:C strain compensation ratio of 8.3. The C concentrations in the four samples were 0, 0.27%, 0.54%, 0.84%. Note that we assume there is

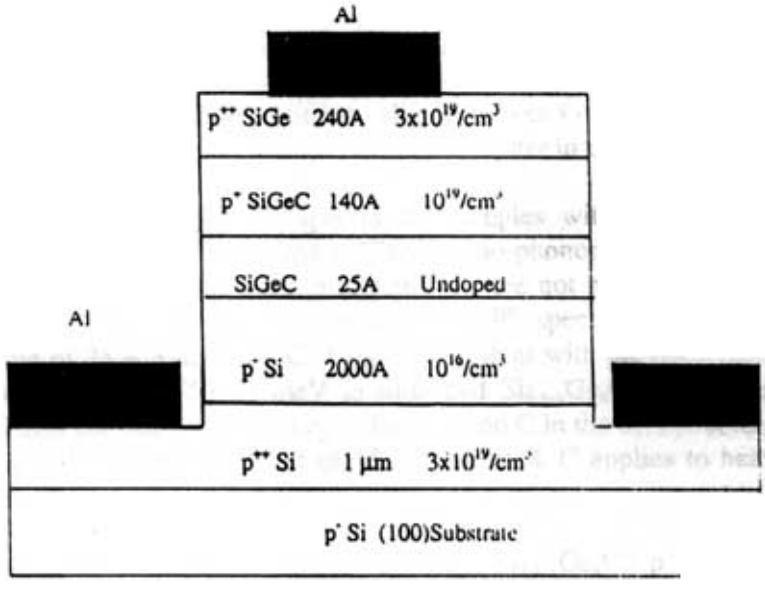

Figure 1: Schematic cross section of the fabricated $p^+ Si_{1-x-y}Ge_xC_y/ p^- Si$ diodes.

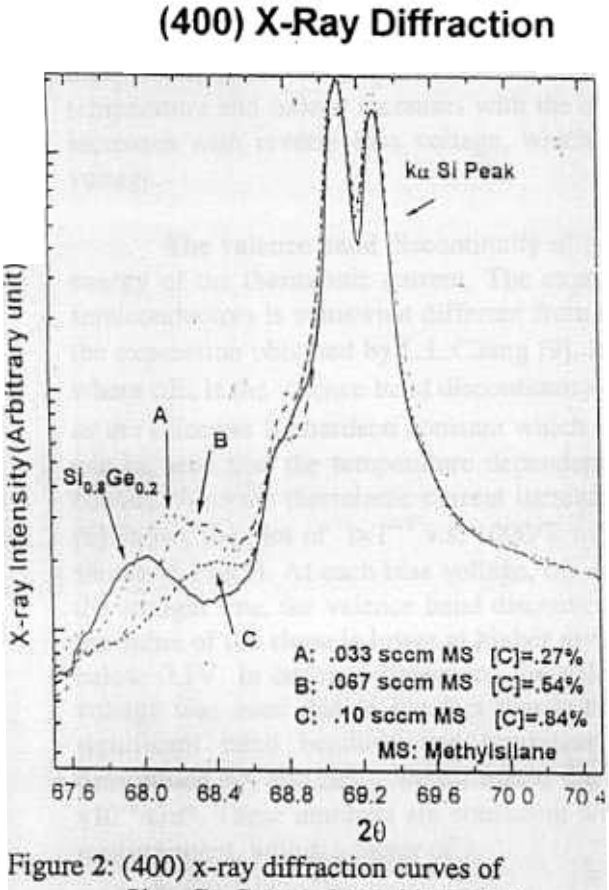

Figure 2: (400) x-ray diffraction curves of $Si_{1-x-y}Ge_xC_y$ samples, with x = 0.2 and various C concentrations. Two peaks in Si substrate come from $K\alpha_1$ and $K\alpha_2$.

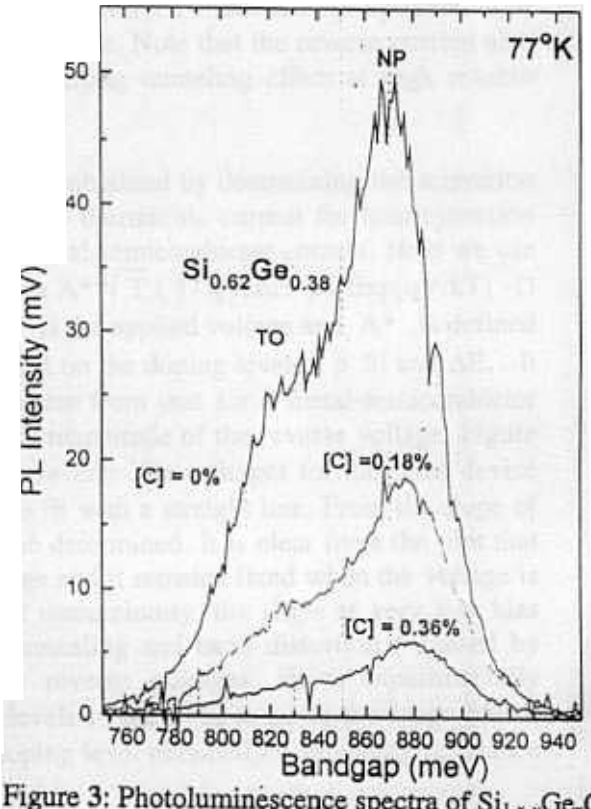

Figure 3: Photoluminescence spectra of $Si_{1-x-y}Ge_xC_y$ samples at 77K, with x=0.38 and two different C concentrations.The pump power is 70 mW/cm^2.

no variation of the Ge concentration as C was added. Evidence of secondary ion mass spectroscopy (SIMS) profiles support this assumption[2]. However, if some of the Ge atoms, as opposed to Si, were replaced by the C atoms, slightly lower Ge and C concentrations would result. We will mention the implication of this assumption later in this paper.

Figure (3) shows the 77K PL spectra for samples with 38% [Ge] and various C concentrations. The samples were measured at 77K. The no-phonon (NP) peak and the transverse optical phonon (TO) replica can be seen, although they are not resolved well due to the band filling effect caused by heavy doping. The peaks of the PL spectra shift to higher energy as C was added, at a rate of 25 ± 3 meV/ % C. This is consistent with previous results showing 1% [C] increases the bandgap by 21-23 meV in **undoped** $Si_{1-x-y}Ge_xC_y$ layers, with x=0.38. The previous work [3] also showed a dependence of bandgap on C in the $Si_{1-x-y}Ge_xC_y$ layers for x=0.2 and x=0.38, so we will assume the result of 25 ± 3 meV/ % C applies to heavily doped $Si_{1-x-y}Ge_xC_y$ with x=0.2.

Shown in Fig (4) is the band structure of the p^+ $Si_{1-x-y}Ge_xC_y$/ p^- Si containing 20% Ge. This structure is the same as the typical HIP structure. The current-voltage characteristics of this device structure are that of a diode. Under forward bias, the hole current coming from the p^- Si will depend on the applied voltage which shifts the valence band structure of the p^- Si relative to that of SiGeC. On the other hand, the hole current under reverse bias will be mostly blocked by the valence band discontinuity of SiGeC/Si. Within a certain temperature range, thermionic emission of holes across the valence band discontinuity will determine the reverse current. Therefore, the hole current would be exponentially dependent on temperature, and measuring the temperature dependence allows one to measure the valence band discontinuity. Figure (5) shows the current-voltage characteristics of the diode containing 20% Ge and 0.84 % of C. The diode rectified at low temperatures. It can be seen that the reverse current is a strong function of temperature and indeed increases with the device temperature. Note that the reverse current also increases with reverse bias voltage, which suggests a strong tunneling effect at high reverse voltage.

The valence band discontinuity of SiGeC/Si was obtained by determining the activation energy of the thermionic current. The expression for the thermionic current for heterojunction semiconductors is somewhat different from that for a metal-semiconductor contact. Here we use the expression obtained by L.L.Chang [9], in which $J = A^* \sqrt{T} (1- qV/\Delta E_v) (Exp[qV/kT] -1)$ where ΔE_v is the valence band discontinuity (in eV); V is the applied voltage and A^* is defined as the effective Richardson constant which is dependent on the doping level in p^- Si and ΔE_v . It can be seen that the temperature dependence is different from that for a metal-semiconductor contact. Also the thermionic current increases with the magnitude of the reverse voltage. Figure (6) shows the plot of $I \times T^{1/2}$ v.s. 1000/T with various reverse bias voltages for the same device shown in Fig(5). At each bias voltage, the data can be fit with a straight line. From the slope of the straight line, the valence band discontinuity can be determined. It is clear from the plot that the value of the slope is lower at higher reverse voltage and it remains fixed when the voltage is below 0.1V. In order to determine the valence band discontinuity, the slope at very low bias voltage was used due to the fact that both carrier tunneling and band distortion (caused by significant band bending) are prominent at high reverse voltages. From experimentally determined A^* and ΔE_v , we estimated the doping levels in the p^- Si to be in the range of 1-2 $x10^{16}$/cm3. These numbers are consistent with the doping level obtained by spreading resistance measurement, within a factor of 3.

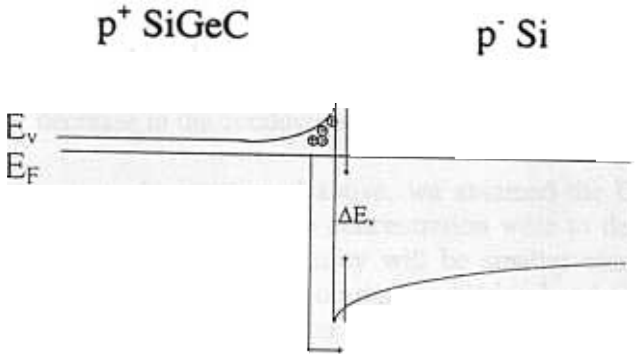

Figure 4: Energy band diagram of p^+ $Si_{1-x-y}Ge_xC_y$/ p^- Si diodes, showing thermally activated leakage current of holes over barrier.

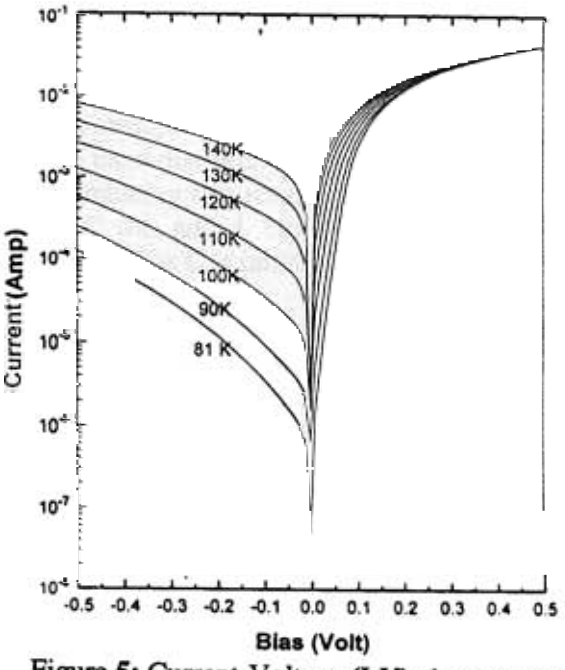

Figure 5: Current-Voltage (I-V) characteristics of p^+ $Si_{1-x-y}Ge_xC_y$/ p^- Si diode at different temperatures. x = 0.20, y = 0.0084.

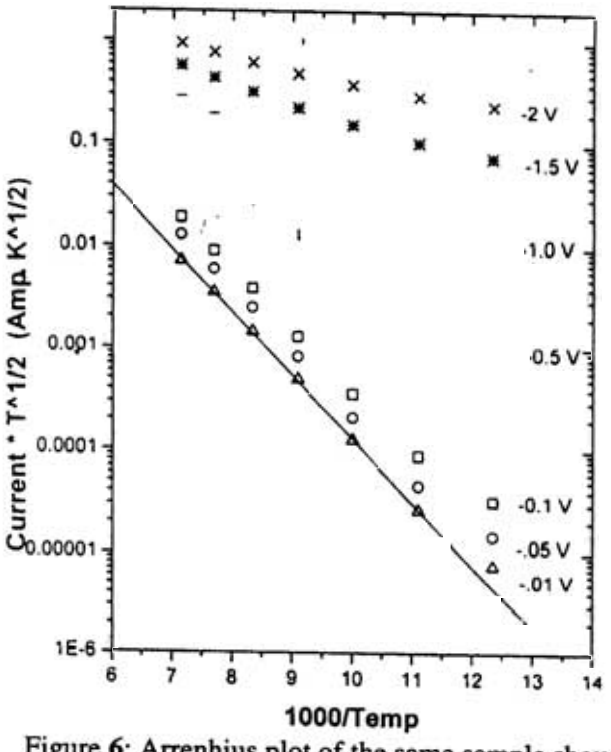

Figure 6: Arrenhius plot of the same sample shown in Fig(5) for various reverse voltages. Valence band discontinuity was obtained by linearly fitting the data at V = -0.01Volt.

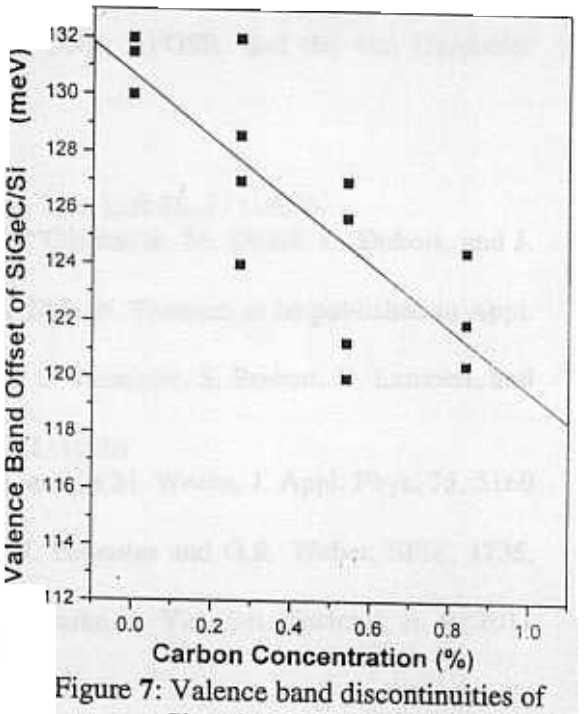

Figure 7: Valence band discontinuities of $Si_{1-x-y}Ge_xC_y$ /Si as a function of C concentrations, with slope equal to 11 meV / % C.

Figure (7) shows the activation energies measured by this method as a function of carbon concentration. Assuming that the fermi level position does not change as a function of C, the best fit slope is -11 ± 2.5 meV/ % C. This implies that the valence band discontinuity between Si and $Si_{1-x-y}Ge_xC_y$ decreases by 11 ± 2.5 meV as C was added. Combining this result with the earlier result of a total bandgap change of 25 ± 3 meV / % C as C was added, our result implies a decrease in the conduction band discontinuity of 14 ± 4 meV / % C as C is initially incorporated.

As mentioned above, we assumed the Ge concentration remains the same when C is incorporated. If the Ge concentration were to decrease as C is added, the carbon effect on the valence band discontinuity will be smaller compared to the 11 meV reduction/ % C result. However, the C effect on the conduction band offset could be the same since Ge concentration has a negligible effect on the conduction band discontinuity with Si.

Conclusion

We have fabricated the p^+ $Si_{1-x-y}Ge_xC_y$/ p^- Si diodes, with x=0.2 and y ranging from 0% to 1%. Results of PL show that 1% C increases the bandgap of p^+ SiGeC alloys by 25 meV, consistent with the result obtained in undoped SiGeC layers. Based on the electrical characterization of leakage currents in these diodes, we have determined that the valence band discontinuities of $Si_{1-x-y}Ge_xC_y$ /Si is reduced as C is added, at a rate of 11 ± 2.5 meV / %C. Combining the change in the band gap and the valence band discontinuity, we can deduce that the conduction band discontinuity of SiGe/Si would decrease by 14 ± 4 meV when 1% C is added.

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