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Direct Optical Measurement of the valence band offset of p^+ $Si_{1-x-y}Ge_xC_y$ / p^- Si (100) by Heterojunction Internal Photoemission

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ABSTRACT

Optical absorption measurements have been performed to study the effect of carbon on the valence band offset of compressively strained p^+ $Si_{1-x-y}Ge_xC_y$/(100) p^- Si heterojunction internal photoemission structures grown by Rapid Thermal Chemical Vapor Deposition (RTCVD) with substitutional carbon levels up to 2.5%. Results indicated that carbon decreased the valence band offset by 26 ± 1 meV/ %C. Results from optical measurement in this study agreed with previous data from capacitance-voltage measurements. Based on previous reports of carbon effect on the bandgap of compressively strained $Si_{1-x-y}Ge_xC_y$, our work suggests that the effect of carbon incorporation on the band alignment of $Si_{1-x-y}Ge_xC_y$/Si is to reduce the valence band offset, with a negligible effect on the conduction band alignment.

INTRODUCTION

Strained $Si_{1-x}Ge_x$/Si heterostructures have been extensively studied and have led to many device applications. The advantage of using strained $Si_{1-x}Ge_x$/Si heterostructures results from the flexibility in bandgap engineering by controlling the amount of incorporated Ge into Si matrix. However, due to the 4% larger atomic size of Ge than that of Si, strain involved in $Si_{1-x}Ge_x$ prevents one from growing unlimited pseudomorphic $Si_{1-x}Ge_x$ layer on Si substrate without introducing misfit dislocations. Recently $Si_{1-x-y}Ge_xC_y$ has attracted a strong interest due to the ability of substitutional C to compensate the strain caused by Ge atoms, with 1% substitutional C compensating the strain caused by 8-10 % Ge [1-6].

Photoluminescence (PL) measurements on $Si_{1-x-y}Ge_xC_y$ as well as transport studies of heterojunction bipolar transistors (HBT's) with $Si_{1-x-y}Ge_xC_y$ as the base showed that the addition of 1% C increases the bandgap of $Si_{1-x}Ge_x$ by 21-26 meV[3-5]. However, reducing the strain in $Si_{1-x}Ge_x$ by adding C increases the bandgap less than does reducing the strain by merely removing Ge. These results imply that, for a given bandgap, $Si_{1-x-y}Ge_xC_y$ has less misfit strain and therefore allows a greater critical thickness than does $Si_{1-x}Ge_x$.

Although it is generally agreed that 1% C increases bandgap by 21~26 meV, it is still under debate regarding how the bandgap increase is allocated in the band alignment of $Si_{1-x-y}Ge_xC_y$ /Si heterostructures. Several electrical and optical methods have been used to determine the band alignment. A temperature-dependent leakage current study on p^+ $Si_{1-x-y}Ge_xC_y$ / p^- Si unipolar diodes indicated that C decreased the valence band offset (ΔE_v) of the resulting $Si_{1-x-y}Ge_xC_y$ /Si heterostructure[13]. However, no accurate quantitative number was extracted due to scatter in data among devices caused by strong dependence of leakage current on local defects. Capacitance-Voltage (C-V) measurements, on the other hand, are theoretically insensitive to anomalous sources of leakage current. They have demonstrated a clear downward trend of ΔE_v of $Si_{1-x-y}Ge_xC_y$ /Si by C incorporation with minimal scatter of data among devices and indicated that

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the increase in bandgap by C is fully accommodated in the valence band[7]. Similar results were also obtained from C-V analysis of $Si_{1-x-y}Ge_xC_y$ based metal-oxide-semiconductor structures[14]. X-ray photoelectron spectroscopy (XPS) evaluation on the $Si_{1-x-y}Ge_xC_y$ /Si valence band offset did not show significant change with carbon incorporation (with accuracy limit ±30 meV), consistent with the finding that the effect of carbon is small[18].

Conflicting results have also been reported. An indirect evidence from PL study on the $Si_{1-x-y}Ge_xC_y$ / $Si_{1-y}C_y$ quantum wells suggested that C increases ΔE_V of $Si_{1-x-y}Ge_xC_y$ /Si by 10 meV/ %C[15]. XPS measurements on Ge-rich $Si_{1-x-y}Ge_xC_y$ indicated an increase in ΔE_V by ~50 meV/%C[19]. Moreover, recent results from admittance spectroscopy on $Si_{1-x-y}Ge_xC_y$/Si multi-quantum wells suggested a large effect by C (~ 80 meV/ %C) on both the conduction and valence band offset of $Si_{1-x-y}Ge_xC_y$ /Si[16]. Given conflicting reports, it is therefore necessary to have a direct optical measurement on the $Si_{1-x-y}Ge_xC_y$ /Si heterostructures. In this study, we report such a measurement of the valence band offset by heterojunction internal photoemission (HIP) of $Si_{1-x-y}Ge_xC_y$/ Si (100) from the onset of photocurrent.

EXPERIMENT

The samples in this study contain 39% Ge and up to 2.5% substitutional carbon and were grown by RTCVD[7]. They contain a p^+ Si buffer for substrate contact, followed by 0.2 μm p^- Si, 2 nm undoped $Si_{1-x-y}Ge_xC_y$ spacer and 18 nm p^+ $Si_{1-x-y}Ge_xC_y$. Finally, a 20 nm heavily doped (~ $10^{20}/cm^3$) Si layer was grown for a top contact. Substitutional carbon fractions were measured by X-ray diffraction, assuming 8.3 Ge/C strain compensation ratio. For the rest of this paper, all carbon levels refer to the substitutional levels measured by this method.

Device were fabricated by a simple mesa etching in CF_4/O_2 plasma and Al metallization by lift-off. A device structure is shown in figure 1. Good rectifying characteristics were observed at low temperatures (~ 77K), indicating a significant valence band offset between p^+ $Si_{1-x-y}Ge_xC_y$ / p^- Si. Samples were further cooled down to ~ 4 K to minimize thermionic leakage current for infrared photocurrent measurements and a good ohmic contact was still observed. Optical absorption measurements were performed at 4K using a calibrated glowbar IR source, a spectrometer and phase-sensitive detection.

Figure 2 shows the band diagram of the p^+ $Si_{1-x-y}Ge_xC_y$ / p^- Si HIP structure. Under a reverse bias, holes current is mostly blocked by the valence band offset and the ideal leakage current comes from thermionically emitted holes from p^+ $Si_{1-x-y}Ge_xC_y$ layer. When infrared light is incident on the p^+ $Si_{1-x-y}Ge_xC_y$ layer, holes will be excited to higher energy states, and if the photon energy is large enough for hole to overcome the barrier posed by the valence band offset, a photocurrent will result. From the band diagram, ΔE_V can be expressed as

$$\Delta E_V = E_{F(SiGeC)} + qV_{bi} + E_{F(Si)} \qquad (1)$$

where $E_{F(SiGeC)}$ is the distance between Fermi level and the valence band of $Si_{1-x-y}Ge_xC_y$, qV_{bi} is the built-in voltage of the junction, $E_{F(Si)}$ is the distance of the valence band of Si and the Fermi level. Since the $Si_{1-x-y}Ge_xC_y$ is heavily doped, the threshold energy for the onset of photocurrent is E_V - $E_{F(SiGeC)}$. To extract ΔE_V, one also needs to know the doping concentrations in $Si_{1-x-y}Ge_xC_y$ to know $E_{F(SiGeC)}$. Doping concentrations were obtained by SIMS measurement on similarly grown samples and SIMS data show no dependence of dopants

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(boron) incorporation on the carbon level. We thus assume the onset of photocurrent tracks accurately with ΔE_V.

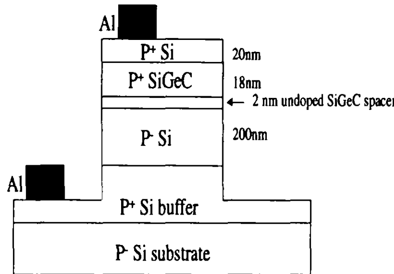

Figure 1: A heterojunction internal photoemission device structure.

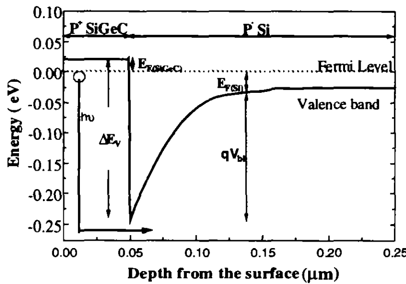

Figure 2: Zero-biased valence band diagram of p^+ $Si_{1-x-y}Ge_xC_y$ /p^- Si.

RESULTS

Figure 3 shows plots of the square root of photoresponse curves as a function of photon energy (Fowler plot) of $Si_{1-x-y}Ge_xC_y$/Si with different carbon concentrations. The onset of photocurrent decreases as carbon level increases, indicating a decreasing ΔE_V with carbon concentrations. Carbon decreases the ΔE_V of $Si_{1-x-y}Ge_xC_y$ / Si by 26±1 meV/%C, as shown in figure 4. This is consistent with previously reported values measured by C-V measurements[7,14], and similar to the increase in bandgap with carbon. We conclude that the increase in bandgap is reflected in the valence band of $Si_{1-x-y}Ge_xC_y$, with very little or no change in the conduction band. Thus little ΔE_c in $Si_{1-x-y}Ge_xC_y$ /Si (100) is expected as in $Si_{1-x}Ge_x$/Si.

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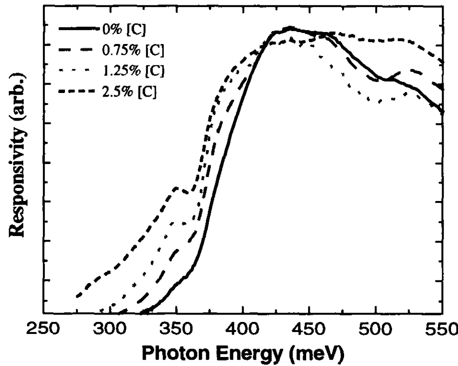
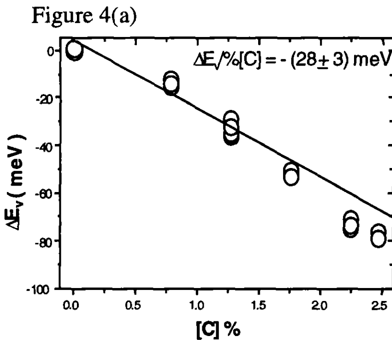


Figure 3: Photoresponse curves of p^+ $Si_{1-x-y}Ge_xC_y$ /p^- Si as well as p^+ $Si_{1-x}Ge_x$/ p^- Si. Samples were measured at 4K.



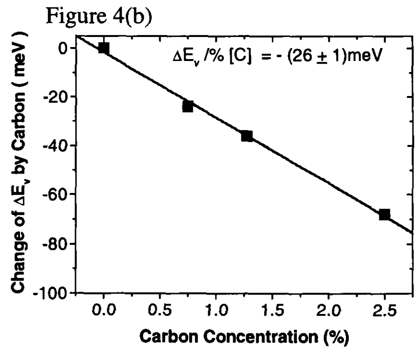


Figure 4: A comparison of change of ΔE_v of $Si_{1-x-y}Ge_xC_y$ /Si as a function of C concentrations. Figure 4(a) is measured by C-V method[7] and figure 4(b) is the results for HIP measurement, as extracted from figure 2.

Figure 5 shows the valence band offset of $Si_{1-x}Ge_x$/Si[18] and $Si_{1-x-y}Ge_xC_y$/Si as a function of lattice mismatch and equivalent Ge levels for $Si_{1-x}Ge_x$ of the given strain. Adding carbon to $Si_{1-x}Ge_x$ to form $Si_{1-x-y}Ge_xC_y$ on silicon (100) reduces both ΔE_V and the compressive strain. But compared to strain reduction by reducing the Ge fraction alone, the ΔE_V reduction by adding carbon is small. For example, the valence band offset of $Si_{0.585}Ge_{0.39}C_{0.025}$ / Si is ~100 meV larger than that of an equally strained $Si_{0.82}Ge_{0.18}$/Si heterostructure. Figure 5 also predicts that,

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by extrapolating the dashed line to the vertical axis, a strain-free $Si_{.563}Ge_{.39}C_{.047}$/Si heterostructure will have ~ 200 meV valence band offset.

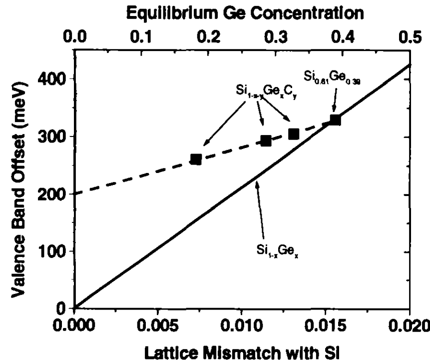

Figure 5: Summary of valence band offsets obtained from optical absorption measurement as a function of lattice mismatch with Si and equivalent Ge concentration. The solid line represents the valence band offsets of $Si_{1-x}Ge_x$/Si.

CONCLUSIONS

In summary, we have studied the valence band offset of compressively strained pseudomorphic $Si_{1-x-y}Ge_xC_y$ /Si (100) by heterojunction internal photomission. Carbon decreased the valence band offset of $Si_{1-x-y}Ge_xC_y$/Si by 26 ± 1 meV/% carbon. Combining this number with previously reported similar increases in the bandgap caused by carbon, we conclude that the band structure of $Si_{1-x-y}Ge_xC_y$ /Si exhibits a large valence band offset and a negligible conduction band offset, similar to that of $Si_{1-x}Ge_x$/Si heterostructures.

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