I. INTRODUCTION

Research on Si/Si$_{1-x-y}$Ge$_x$$_y$ heterostructure materials and devices has led to dramatic improvements in performance and functionality of Si-based electronic and optoelectronic devices. For example, Si/Si$_{1-x-y}$Ge$_x$$_y$ heterojunction bipolar transistors have been fabricated with a power gain cutoff frequency, $f_{max}$, of 160 GHz$^2$ and with a current gain cutoff frequency, $f_t$, of 113 GHz.$^2$ Additionally, improvements in both the transconductances and the mobilities in both $p$-channel$^3$ and $n$-channel$^4$ heterojunction field-effect transistors with Si$_{1-x-y}$Ge$_x$$_y$ based materials have been demonstrated. However, the 4.18% lattice mismatch between Si and Ge imposes significant restrictions on composition and layer thickness in Si/Si$_{1-x-y}$Ge$_x$$_y$ heterostructures.

Recently, considerable progress has been made in the growth and characterization of Si$_{1-x-y}$Ge$_x$$_y$ alloys,$^5$–$^{11}$ which offer considerably greater flexibility, compared to that in the Si/Si$_{1-x-y}$Ge$_x$$_y$ material system, to control strain and electronic properties in group IV heterostructures. In particular, the smaller C atom compensates for the compressive strain present in Si$_{1-x-y}$Ge$_x$$_y$, leading to the possibility of fabricating group IV heterostructures lattice matched to Si substrates.$^5$–$^{11}$ Recent measurements of the total energy band gap for Si$_{1-x-y}$Ge$_x$$_y$ compressively strained to Si (001) indicate that incorporation of C into Si$_{1-x-y}$Ge$_x$$_y$ increases the band gap by 21–26 meV/% C.$^{12}$–$^{15}$ Effective design, fabrication, and characterization of such devices, however, additionally requires the accurate measurement of the energy band offsets in Si/Si$_{1-x-y}$Ge$_x$$_y$ heterostructures. Moreover, determining the effects of nonsubstitutional C on the electronic structure of these alloys is another key step to realizing these devices.

Although measuring energy band offsets presents many challenges to the experimentalist, admittance spectroscopy has been used successfully on several material systems in the past.$^{16}$–$^{18}$ In this article we present admittance spectroscopy measurements of valence- and conduction-band offsets, $\Delta E_v$ and $\Delta E_c$, respectively, in Si/Si$_{1-x-y}$Ge$_x$$_y$ heterostructures. A detailed description of the technique can be found elsewhere.$^{19}$ Since many of the samples examined contain a substantial fraction of nonsubstitutional C (0.29–1.6 at. %), we also examined some of these samples using deep-level transient spectroscopy in an effort to gain an understanding of the influence of nonsubstitutional C on the electronic structure of these alloys.

II. EXPERIMENT

Several multiple quantum well (MQW) samples were grown by solid-source molecular beam epitaxy (MBE) on Si (001) conducting substrates (see Table I). The epilayers consisted of a 2000 Å Si buffer layer, followed by 150–250 Å of Si$_{1-x-y}$Ge$_x$$_y$ or Si$_{1-x-y}$Ge$_x$$_y$$_y$$_y$$_y$$_y$, alternating with 350 Å Si for ten periods with dopant concentrations of $7.4 \times 10^{16}$ and $1 \times 10^{17}$ cm$^{-3}$, respectively. Either $p$-type (B-doped) or
n-type (Sb-doped) structures were used for measurement of, respectively, $\Delta E_v$ and $\Delta E_c$. The heterostructures were grown at 450 °C, with some capped by an additional 2000 Å Si. Several samples were grown using Sb as a surfactant to improve structural quality.\(^{21}\) In all cases the thickness of the MQW structure was below the critical thickness for strain relaxation.\(^{22}\) X-ray diffraction (XRD), ion channeling, and, in some cases, transmission electron microscopy (TEM) were performed to confirm the high structural quality of the samples. The Ge concentration was determined using Ruthenford backscattering, and the C concentration was then determined by applying a strain compensation ratio for Ge:C of 9.44:1, which is given by a linear interpolation of lattice constants between Si, Ge, and 3C-SiC, to the XRD patterns. In addition, secondary ion mass spectroscopy was used to determine the total C concentration.

Schottky barrier diodes required for the admittance measurements were formed by deposition of Cr/Au circular contacts 150–300 μm in diameter, followed by a mesa etch in a CF$_4$/O$_2$ plasma. A schematic energy band diagram for an n-type Si/Si$_{1-x}$Ge$_x$ MQW structure is shown in Fig. 1(a). Al Ohmic contacts were then deposited on the back-sides of the samples.

In addition, several Si/Si$_{1-x}$Ge$_x$C$_y$ heterostructures were grown by chemical vapor deposition (CVD) in a single wafer reactor on Si (001) conducting substrates. These samples consisted of a 500 Å $p$-type Si buffer layer, a 300 Å $p$-type Si$_{1-x}$Ge$_x$ single quantum well (SQW), a 2000 Å $p$-type Si spacer, and finally a 600 Å $n$-type Si cap [see the energy band diagram in Fig. 1(b)]. All the layers had dopant concentrations of approximately $1 \times 10^{17}$ cm$^{-3}$, except the cap which had a dopant concentration of $5 \times 10^{18}$ cm$^{-3}$. Extensive characterization of previous growths provided an accurate calibration of the Ge and C concentrations. Since a $pn$ junction is used to perform the admittance spectroscopy on these samples, 300 μm diameter circular Al Ohmic contacts were deposited on the top sides of these samples followed by a mesa etch and an Al Ohmic backside contact.

### III. RESULTS AND DISCUSSION

#### A. Admittance spectroscopy

We first examined several $p$-type Si/Si$_{1-x}$Ge$_x$ heterostructures to verify the validity of the measurement technique (see samples MBE-1–3 in Table I). Valence-band (VB) offsets measured for these Si/Si$_{1-x}$Ge$_x$ were found to be in excellent agreement with accepted values.\(^{23,24}\) Admittance measurements were then performed on various Si$_{1-x}$Ge$_x$C$_y$ heterostructures. Figure 2 shows the conductance and capacitance measured as functions of temperature for various frequencies for sample CVD-1. Conductance peaks and capacitance steps arising from temperature-dependent thermionic emission from the quantum well are clearly observed. The inset in Fig. 2 shows an Arrhenius plot of $f$ and $T_m$, from which an activation energy of 68 ± 19 meV is obtained. The VB offset derived from this activation energy\(^{19}\) was found to be 88 ± 20 meV.

Similar measurements were performed on the other heterostructures, and a summary of the results can be seen in Fig. 3 and Table I. As shown in Fig. 3, incorporation of C into Si$_{1-x}$Ge$_x$C$_y$ lowers both the conduction-band- and the

### Table I. Summary of results for Si/Si$_{1-x}$Ge$_x$ and Si/Si$_{1-x}$Ge$_x$C$_y$ heterostructures analyzed.

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Type</th>
<th>Ge conc. (at. %)</th>
<th>Subst. C conc. (at. %)</th>
<th>Total C conc. (at. %)</th>
<th>Sb surf.?</th>
<th>Measured band offset (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MBE-1</td>
<td>$p$</td>
<td>10.6%</td>
<td>0%</td>
<td>N/A</td>
<td>No</td>
<td>$\Delta E_v$ = 108 ± 20</td>
</tr>
<tr>
<td>MBE-2</td>
<td>$p$</td>
<td>17.9%</td>
<td>0%</td>
<td>N/A</td>
<td>No</td>
<td>$\Delta E_v$ = 160 ± 20</td>
</tr>
<tr>
<td>MBE-3</td>
<td>$p$</td>
<td>25.5%</td>
<td>0%</td>
<td>N/A</td>
<td>No</td>
<td>$\Delta E_v$ = 198 ± 12</td>
</tr>
<tr>
<td>MBE-4</td>
<td>$P$</td>
<td>20.6%</td>
<td>0.44%</td>
<td>0.48%</td>
<td>No</td>
<td>$\Delta E_v$ = 118 ± 12</td>
</tr>
<tr>
<td>MBE-5</td>
<td>$p$</td>
<td>39.4%</td>
<td>1.14%</td>
<td>?</td>
<td>Yes</td>
<td>$\Delta E_v$ = 223 ± 20</td>
</tr>
<tr>
<td>MBE-6</td>
<td>$n$</td>
<td>16.9%</td>
<td>1.14%</td>
<td>2.80%</td>
<td>Yes</td>
<td>$\Delta E_v$ = 100 ± 15</td>
</tr>
<tr>
<td>MBE-7</td>
<td>$n$</td>
<td>23.4%</td>
<td>2.21%</td>
<td>3.62%</td>
<td>Yes</td>
<td>$\Delta E_v$ = 275 ± 23</td>
</tr>
<tr>
<td>MBE-8</td>
<td>$n$</td>
<td>9.3%</td>
<td>0.81%</td>
<td>1.10%</td>
<td>Yes</td>
<td>No peaks</td>
</tr>
<tr>
<td>MBE-9</td>
<td>$n$</td>
<td>29.3%</td>
<td>2.37%</td>
<td>4.21%</td>
<td>Yes</td>
<td>$\Delta E_v$ = 149 ± 21</td>
</tr>
<tr>
<td>CVD-1</td>
<td>$n$</td>
<td>30%</td>
<td>1.50%</td>
<td>?</td>
<td>No</td>
<td>$\Delta E_v$ = 88 ± 20</td>
</tr>
<tr>
<td>CVD-2</td>
<td>$p$</td>
<td>25%</td>
<td>1.25%</td>
<td>?</td>
<td>No</td>
<td>$\Delta E_v$ = 59 ± 17</td>
</tr>
<tr>
<td>CVD-3</td>
<td>$p$</td>
<td>25%</td>
<td>1.50%</td>
<td>?</td>
<td>No</td>
<td>$\Delta E_v$ = 43 ± 11</td>
</tr>
</tbody>
</table>
valence-band-edge energies compared to those for pure Si$_{1-x}$Ge$_x$, while slightly increasing the total band gap. Comparisons of our measured Si/Si$_{1-x-y}$Ge$_x$C$_y$ band offset values with reported results for the change in total energy band gap, $\Delta E_g$, of 21–26 meV/% C (substitutional C) for Si$_{1-x-y}$Ge$_x$C$_y$ compressively strained to Si (001)$^{12-15}$ indicates that the band alignment for our samples is type I. Furthermore, these comparisons show that our band offset values are in quantitative agreement with reported values for $\Delta E_g$ over the range of compositions for which we have measured the band offsets. Combining our average change in $\Delta E_g$, 107±6 meV/% C, with our average change in $\Delta E_c$, 75±6 meV/% C, we obtain a value for the change in band gap, $\Delta E_g$, of 32±9 meV/% C (for substitutional C). One of the samples, MBE-7, exhibits a significantly stronger dependence of $\Delta E_g$ on C concentration than do the others. This sample, however, contains a large C concentration, 2.21 at. % substitutional and 3.63 at. % total, and this anomalous dependence may arise partly from the presence of a particularly high concentration of nonsubstitutional C.

We may extrapolate our measured band offsets to a wider range of Ge and C composition using the model-solid approach described by Van de Walle.$^{25}$ Using this approach, which systematically incorporates both the compositional or ‘‘alloy’’ contribution and the strain effect on the band offset, we have confirmed that our measured value of $\Delta E_g$ is in agreement with estimates of Si/Si$_{1-x-y}$C$_y$ conduction-band offsets obtained from electrical and photoluminescence$^{26}$ measurements. $C-V$ measurements$^{27}$ on Si/Si$_{1-x-y}$C$_y$ metal-oxide-semiconductor field-effect transistor structures yielded $\Delta E_g$ = 40 meV for Si/Si$_{0.998}$C$_{0.004}$ and $\Delta E_g$ = 70 meV for Si/Si$_{0.992}$C$_{0.008}$. In comparison, our measurements would indicate values of 52±18 meV and 106±22 meV, respectively. Hall measurements$^{28}$ on a Si/Si$_{0.992}$C$_{0.02}$ QW suggest a lower bound on the CB offset of 150 meV; our results correspond to a CB offset of 261±14 meV.

**B. Deep-level transient spectroscopy**

Using the notation $E(x)$ to denote an electron trap level at energy $E_{c} - x$ eV, C has been found to form several electron traps in Si, including an interstitial $C_i$ level at $E(0.12)^{29}$ and a $C_T$-Si pair at $E(0.17)$. As shown in Table I, many of the samples contain a significant fraction of C incorporated nonsubstitutionally. Deep-level transient spectroscopy (DLTS) was performed on several of the samples to assess the impact of this nonsubstitutional C on the electronic structure of Si$_{1-x-y}$Ge$_x$C$_y$ alloys. Interpretation of the spectra is complicated by the presence of the quantum wells because, under certain measurement conditions, one would expect emission from the wells to display itself as a DLTS peak. For all of the measurement conditions we have used, there were no DLTS peaks at the activation energy corresponding to the peaks in the admittance spectra, indicating that we are in fact observing deep-level traps. DLTS spectra from sample MBE-6 that was obtained for $V_{pp} = -1$ V, $V_{pulse} = -0.1$ V, a pulse width of 1 ms, and various rate windows is shown in Fig. 4. We observe three clear deep levels corresponding to electron traps at $E1(0.231±0.020)$, $E2(0.334±0.008)$, and $E3(0.405±0.012)$. The largest of these peaks corresponds to a trap concentration of approximately $2 \times 10^{11}$ cm$^{-3}$. There also appear to be several minor peaks within the spectrum, but accurate activation energies could not be extracted. In sample MBE-8, for which no peaks in the admittance spectra...
were observed, we observed a single DLTS peak that corresponds to an electron trap at E4(0.356 ± 0.023).

A large number of deep levels have been identified in Si and Si1−xGex by deliberately incorporating a known impurity,31 by deliberately damaging the sample using etching32 or radiation bombardment,33 or by combining DLTS with other measurements, such as electron paramagnetic resonance.34 Although additional measurements have not been performed on these samples, we have identified in the literature some possibilities for the sources of these traps. For Si1−xGex, previously reported measurements of the compositional behavior of the trap energy levels suggest that the energy levels are pinned to an absolute reference energy, thereby displaying a shift in measured activation energy equal in amount to the shift in the relevant band edge.

Therefore, we have used the model-solid approach to shift our measured levels by the expected value for ΔEc, which is 107±16 meV for MBE-6 and 72±11 meV for MBE-8. When this calculation is performed, we are left with deep-levels at E1(0.338±0.026), E2(0.441±0.018), and E3(0.512±0.020) for sample MBE-6 and E4(0.428±0.025) for sample MBE-8. The traps E2 and E4 in the two samples now appear to be due to the same defect level at 437 ± 15 meV below the conduction-band edge of Si, a level that is consistent with a Sb vacancy pair level previously observed in Si1−xGex.37 The E1 level may be due to an oxygen-related defect38 or a dislocation kink site,35 and the E3 level, which we have also observed in much lower densities (∼5 × 10^{12} cm^{-3}) in similar Si/Si1−xGe heterostructures, could be due to a Au-related defect39 or to an unidentified midgap recombination-generation center.35

Interestingly, the shallow interstitial C levels mentioned earlier are not observed at the expected temperatures (below 100 K) to a sensitivity of ∼2 × 10^{13} cm^{-3} in samples MBE-6 and MBE-8, even though they contain, respectively, 1.7 at. % and at. 0.4 at. % nonsubstitutional C. If the levels remain fixed with respect an absolute reference energy, then we would not expect to observe them in the DLTS signal because the conduction-band edge itself is close to or below the E(0.12) and E(0.17) levels. It is possible in fact that the nonsubstitutional C contributes additional states above the conduction-band edge of Si1−xGeC_y, thereby adding to the density of states within the quantum wells.

**IV. CONCLUSION**

Admittance spectroscopy and deep-level transient spectroscopy have been performed to elucidate the electronic structure of Si/Si1−x,yGeC_6 heterostructures. Both the conduction- and valence-band offsets have been extracted from the admittance spectra, and both band-edge energies were observed to decrease, compared to those of pure Si1−xGe_x. The resulting conduction-band offsets may allow SiSi1−x,yGeC_6 or Si/Si1−x,yC heterojunctions to provide an attractive alternative to Si/Si1−x,yC heterostructures. DLTS measurements have revealed the presence of a number of deep electron traps in Si1−x,yGeC_6 alloys. Previously reported interstitial C levels were not observed, despite the presence of a substantial fraction of nonsubstitutional C. Work is currently in progress to further characterize the effects of this nonsubstitutional C on the electronic structure of these alloys.

**ACKNOWLEDGMENTS**

The authors would like to thank M. Robinson, J. E. Huffman, and R. Westhoff at Lawrence Semiconductor Research Laboratory for growth of the CVD samples. The authors would like to acknowledge support from DARPA MDA972-95-3-0047 for work at UCSD, HRL, ASU, and LSRL and from ONR Grant No. N00014-95-1-0996 for work at UCSD. E.T.Y. would like to acknowledge receipt of a Sloan Research Fellowship. B.L.S. and E.T.Y. would also like to thank S. S. Lau for access to part of the equipment used in this work.

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