Deep-level transient spectroscopy of $Si/Si_{1-x-y}Ge_xC_y$ heterostructures

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Deep-level transient spectroscopy was used to measure the activation energies of deep levels in *n*-type $Si/Si_{1-x-y}Ge_xC_y$ heterostructures grown by solid-source molecular-beam epitaxy. Four deep levels have been observed at various activation energies ranging from 231 to 405 meV below the conduction band. The largest deep-level concentration observed was in the deepest level and was found to be approximately 2×10^{15} cm^{-3}. Although a large amount of nonsubstitutional C was present in the alloy layers (1–2 at. %), no deep levels were observed at any energy levels that, to the best of our knowledge, have been previously attributed to interstitial C. © *1998 American Institute of Physics.* [S0003-6951(98)01631-3]

Recently, substantial improvements in the growth of $Si_{1-x-y}Ge_xC_y$ alloys have generated great interest in $Si/Si_{1-x-y}Ge_xC_y$ heterostructure devices.[1–3] One reason for this interest is the considerably greater flexibility, compared to that available in the $Si/Si_{1-x}Ge_x$ material system, to control strain and electronic properties in group IV heterostructure materials, as well as the possibility offered by $Si_{1-x-y}Ge_xC_y$ alloys of fabricating heterostructure devices lattice matched to Si substrates.[1–3] Recent measurements of the total-energy band gap for $Si_{1-x-y}Ge_xC_y$ compressively strained to Si (001) indicate that incorporation of C into $Si_{1-x-y}Ge_xC_y$ increases the band gap by 21–26 meV/%C.[4–7] Additional measurements have shown a reduction in $Si/Si_{1-x-y}Ge_xC_y$ valence-band offset[8–10] and an increase in conduction-band offset with C incorporation into $Si_{1-x-y}Ge_xC_y$ alloys under compressive strain.[10] This increased conduction-band offset may offer an alternative to $Si/Si_{1-x}Ge_x$ grown on strain-relaxed $Si_{1-x}Ge_x$ buffer layers for fabrication of *n*-type heterostructure devices. Realization of such devices, however, requires a greater understanding of the effect of C on both the electronic and the structural properties of these materials. In particular, characterizing the deep-level states present in $Si_{1-x-y}Ge_xC_y$ alloy layers is an important step in refining our understanding of the role C plays in altering the electronic structure of the alloy.

In this letter we present results of deep-level transient spectroscopy (DLTS) performed on *n*-type $Si/Si_{1-x-y}Ge_xC_y$ and $Si/Si_{1-x}Ge_x$ heterostructures. Multiple-quantum-well (MQW) samples were grown by solid-source molecular-beam epitaxy on *n*-type ($\rho<0.007\,\Omega$ cm) Si (100) substrates, and consisted of 150–250 Å $Si_{1-x-y}Ge_xC_y$ or $Si_{1-x}Ge_x$ alternating with 350 Å Si for ten periods with dopant concentrations of 7.4×10^{16}–1×10^{17} cm^{-3}. These heterostructures were grown at a substrate temperature of 450 °C on 2000 Å Si buffer layers, using Sb as a surfactant to improve structural quality.[11] In all cases the thickness of the MQW structure was below the critical thickness for strain relaxation.[12] Schottky barrier diodes required for the DLTS measurements were formed by deposition of Cr/Au circular contacts 300 μm in diameter, followed by a mesa etch in a CF_4/O_2 plasma. Ohmic contacts were then formed by deposition of Al on the backsides of the samples.

X-ray diffraction, ion channeling, and transmission electron microscopy were performed on these samples, indicating good structural quality in both samples. The Ge concentration was determined using Rutherford backscattering, and the substitutional C concentration was then determined by applying a strain compensation ratio for Ge:C of 9.44:1, which corresponds to a linear interpolation of lattice constants between Si, Ge, and SiC, to the x-ray diffraction spectra. In addition, secondary ion mass spectrometry (SIMS) was used to determine the total C concentration. Comparison of the x-ray diffraction and SIMS data for these samples indicated the presence of a substantial concentration of nonsubstitutional C, with total and substitutional C concentrations of 2.8 and 1.1 at. %, respectively, determined for sample A and 1.1 and 0.8 at. %, respectively, determined for sample B.

Interpretation of the DLTS spectra performed on such an MQW structure is complicated by the presence of the quantum wells because if the measurement parameters are such that capture and emission from the wells is observed, the signal may take the form of a giant ''trap'' due to the wells. The conduction-band offset for the $Si/Si_{0.82}Ge_{0.169}C_{0.011}$ MQW structure, determined by admittance spectroscopy re-

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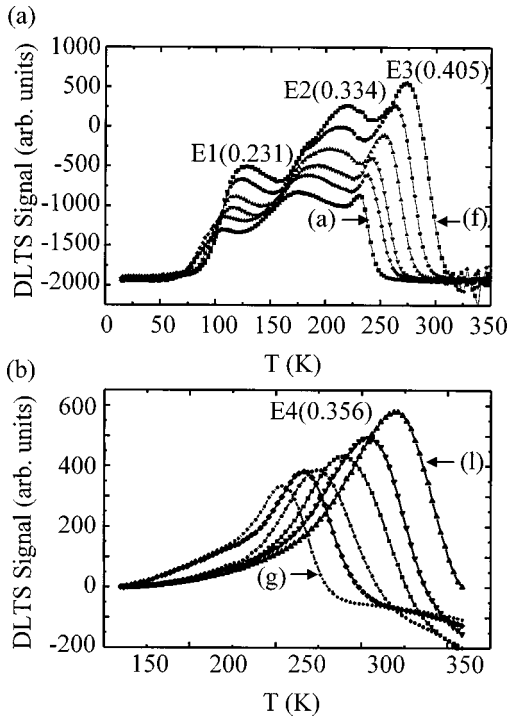

FIG. 1. DLTS spectra for two *n*-type MQW structures: (a) $Si/Si_{0.82}Ge_{0.169}C_{0.011}$ (sample A) with $V_{rev}=-1.0$ V, $V_{pulse}=-0.1$ V, a pulse width of 1 ms, and rate windows of 20, 50, 80, 200, 400, and 1000 Hz for (a)–(f), respectively, and (b) $Si/Si_{0.899}Ge_{0.093}C_{0.008}$ (sample B) with $V_{rev}=-1.0$ V, $V_{pulse}=-0$ V, a pulse width of 1 ms, and rate windows of 20, 50, 80, 200, 400, and 1000 Hz for (g)–(l), respectively.

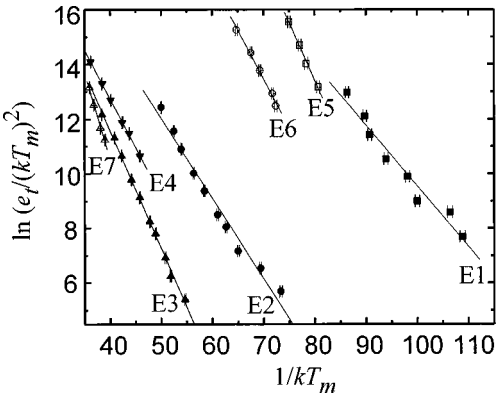

FIG. 2. Arrhenius plots of $\ln(e_t/(kT_m)^2)$ and $1/kT_m$, where e_t is the thermal emission time given by the rate window of the measurement at the peak temperature T_m. The closed symbols represent peaks for the $Si/Si_{1-x-y}Ge_xC_y$ MQW structures, and the open symbols represent peaks for the $Si/Si_{0.8}Ge_{0.2}$ MQW structure.

sults reported elsewhere, was found to be 100 ± 11 meV.[13] No DLTS peak corresponding to this energy was observed, indicating that emission from the well was not contributing to the capacitance signal for our DLTS measurement conditions. No peaks were observed in the admittance spectra of the $Si/Si_{0.896}Ge_{0.093}C_{0.011}$ MQW structure, but previous band-offset measurements for $Si/Si_{1-x-y}Ge_xC_y$ heterojunctions[10,13] suggest that the conduction-band offset at this composition would be small (72 ± 11 meV), and therefore, difficult to observe experimentally.

Figure 1(a) shows the DLTS spectrum for the $Si/Si_{0.82}Ge_{0.169}C_{0.011}$ sample, clearly revealing the presence of several deep levels. Using the notation $E(x)$ for a deep level at E_c-x eV, the three most clearly discernible levels and their corresponding activation energies are E1(0.231 ±0.02), E2(0.334 ± 0.008), and E3(0.405 ± 0.012). A small peak in the spectrum is visible near 70 K, but the peak intensity was not sufficient to allow extraction of an accurate activation energy. Data for this sample were obtained for temperatures as low as 10 K, and no peaks were observed at lower temperatures that might correspond to shallower levels, to within a sensitivity of $\sim2\times10^{13}$ cm^{-3}, which is limited by a relatively high doping in these heterostructures. Because the peak height is proportional to the density of states of the level, the quantum wells would have a much larger signal than our sensitivity limit if they were contributing to the capacitance transients. Figure 1(b) shows DLTS spectra for the $Si/Si_{0.896}Ge_{0.093}C_{0.011}$ MQW structure. A deep level E4 is observed, with an activation energy of 0.356 ±0.023 eV. Arrhenius plots for all four of these levels are shown in Fig. 2, and a summary of these results is given in Table I.

A large number of deep levels have been identified in Si and $Si_{1-x}Ge_x$ using various other techniques in conjunction with DLTS.[14–17] Although additional measurements have not been performed on these samples, we have identified in the literature some possibilities for the sources of these deep levels. First-principles self-consistent electronic structure calculations have revealed that many deep impurity levels are expected to be invariant in energy with respect to an absolute vacuum level.[18] For $Si_{1-x}Ge_x$, previously reported measurements of the compositional behavior of deep-level energies have shown that often levels are, in fact, pinned to the vacuum energy level, thereby displaying a shift in measured activation energy equal to the shift in the relevant band-edge energy.[19,20] Based on experimentally measured values for the conduction-band offsets in $Si/Si_{1-x-y}Ge_xC_y$ heterostructures,[12] we expect conduction-band offsets of 107 ± 16 and 72 ± 11 meV for $Si/Si_{0.82}Ge_{0.169}C_{0.011}$ and $Si/Si_{0.896}Ge_{0.093}C_{0.011}$, respectively. Using these band-offset values, we obtain deep-level energies, referred to the Si conduction-band edge, shown in Table I. Levels 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 an Sb–vacancy pair level previously observed in $Si_{1-x}Ge_x$ doped with Sb.[21] The presence

TABLE I. Summary of heterostructure compositions and deep levels measured by DLTS.

Sample	(Ge)	Total (C)	Subst. (C)	Activation energy of observed deep levels	Shifted trap energies (referred to Si conduction-band edge)
A	16.9%	2.8%	1.1%	E1(0.231), E2(0.334), E3(0.405)	E1(0.338), E2(0.441), E3(0.512)
B	9.3%	1.1%	0.8%	E4(0.356)	E4(0.428)
C	20%	0%	0%	E5(0.353), E6(0.465), E7(0.639)	E5(0.353), E6(0.465), E7(0.639)

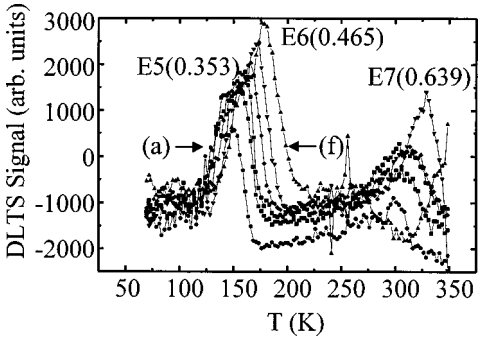

FIG. 3. DLTS spectra for an *n*-type $Si/Si_{0.8}Ge_{0.2}$ MQW structure, with $V_{rev}=-4.0$ V, $V_{pulse}=-0.1$ V, a pulse width of 1 ms, and rate windows of 20, 50, 80, 200, 400, and 1000 Hz for (a)–(f), respectively.

of this defect level in our samples is not unexpected given the use of Sb as a surfactant during growth and as a dopant in the MQW structure. The E1 level may be due to an oxygen-related defect[22] or a dislocation kink site,[19] and the E3 level, which we have also observed in much lower densities ($<\sim 5\times10^{12}$ cm^{-3}) in similar $Si/Si_{1-x}Ge_x$ heterostructures, could be due to a Au-related defect[23] or to an unidentified midgap recombination–generation center.[19]

For comparison, DLTS measurements were also performed using a nominally undoped $Si/Si_{0.8}Ge_{0.2}$ MQW structure grown under conditions very similar to those used during the growth of the $Si/Si_{1-x-y}Ge_xC_y$ structures, including the Sb surfactant. The low dopant concentration in this sample ($\sim 1\times10^{15}$ cm^{-3} as determined by capacitance–voltage profiling) yielded much improved sensitivity in the DLTS measurements compared to that attainable for the $Si/Si_{1-x}Ge_xC_y$ structures. Figure 3 shows a DLTS spectrum for the $Si/Si_{0.8}Ge_{0.2}$ MQW structure. Three deep levels are observed, with activation energies $E5(0.353\pm0.019)$, $E6(0.465\pm0.025)$, and $E7(0.639\pm0.037)$, and Fig. 2 shows the Arrhenius plots for these peaks. The largest peak corresponds to a concentration of $\sim 3\times10^{12}$ cm^{-3}. The lower concentration of these levels in the $Si/Si_{1-x}Ge_x$ samples as compared with the $Si/Si_{1-x-y}Ge_xC_y$ heterostructures suggests that these levels are not processing induced. Level E5 corresponds closely in energy to level E1 observed in the $Si/Si_{1-x}Ge_xC_y$ structures, while E6 is very close in energy to the E2/E4 Sb–vacancy pair level. Level E7 may correspond to a midgap recombination–generation center, but the source of this center is less certain.

Despite the presence of a high concentration of nonsubstitutional C in the $Si/Si_{1-x}Ge_xC_y$ samples as indicated in Table I, we do not observe any deep levels corresponding to previously reported electron traps in Si associated with nonsubstitutional C. C has been found to form several electron traps in Si, most notably an interstitial C_i level at 0.12 eV below E_c (Ref. 24) and a C_i–Si pair at 0.17 eV below E_c.[25] Neither of these levels are observed at the expected temperatures (below $\sim$100 K) in our $Si/Si_{1-x}Ge_xC_y$ samples down to a sensitivity of $\sim 2\times10^{13}$ cm^{-3}. Nonsubstitutional C has also been reported to form hole traps in Si at energy levels $E_v+0.30$ and $E_v+0.36$ eV. Such hole traps would not have been observed in our studies, which included only majority-carrier measurements on *n*-type samples. Another possibility is that at these large nonsubstitutional C concentrations, the high concentration of relatively shallow levels at $E_c-0.12$ eV may form an impurity band, merge into the conduction band, or become too shallow to measure using DLTS.

In conclusion, deep-level transient spectroscopy measurements were performed on $Si/Si_{1-x-y}Ge_xC_y$ and $Si/Si_{1-x}Ge_x$ MQW heterostructures to characterize the influence of C on the electronic structure of these alloys. These measurements have revealed the presence of a number of deep levels in $Si_{1-x-y}Ge_xC_y$ alloys. Possible physical origins for these deep levels have been identified based on a comparison of our measured activation energies with those for previously identified deep levels in Si. Previously reported interstitial C electron trap levels were not observed, despite the presence of a substantial fraction of nonsubstitutional C in these samples.

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