Deep photoluminescence in Si/Si$_{1-x}$Ge$_x$/Si quantum wells created by ion implantation and annealing

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Strong broad photoluminescence similar to that observed in some materials grown by molecular beam epitaxy (MBE) has been observed in Si/Si$_{1-x}$Ge$_x$/Si quantum wells grown by chemical vapor deposition. As grown, the samples exhibited SiGe band-edge phonon-resolved bound-exciton luminescence, but after being self-implanted with silicon and annealed at 600 °C, a deep broad luminescence band 80–100 meV below the excitonic gap was observed. This strong luminescence disappeared with an 800 °C anneal and had a pump power and temperature dependence similar to that observed in MBE samples. This is the first time that such luminescence has been observed in material other than that grown by MBE.

In strained Si$_{1-x}$Ge$_x$ quantum wells and superlattices on Si (100) substrates, two basic types of luminescence have been observed: sharp phonon-resolved band-edge exciton luminescence, and/or a deeper broad luminescence band which we shall refer to as the MBE band, since the latter is often observed in samples grown by solid-source molecular beam epitaxy (MBE).[1–4] The former is usually observed in samples grown by chemical vapor deposition (CVD),[5–7] and has also been observed in some samples grown by MBE, particularly in very thin wells or in samples grown at high temperature (⩾600 °C).[3,4,8–11] The physical origin of this deep broad luminescence band is controversial, and theories include an optically active defect,[2] Ge-rich platelets,[9] and donor–acceptor pairs.[12] In this letter, we describe how the luminescence mechanism in CVD samples can be switched from bound excitons to a broad band luminescence similar to that seen in MBE samples, and back again, by ion implantation and annealing.

The samples used in this study were single Si$_{1-x}$Ge$_x$ layers with silicon caps, grown by rapid thermal CVD on (100) silicon substrates, similar to those in Ref. 13. The Si$_{1-x}$Ge$_x$ layers were grown at 625 °C (except 700 °C for $x \leqslant 0.1$) on top of a high-temperature (1000 °C) silicon buffer layer and were followed by a 15 nm Si cap layer grown at 700 °C. For this study, three samples were used. Sample 733 had an atomic Ge fraction of $x=0.20$ and a SiGe width of ~6 nm; 746 had $x=0.25$ and a SiGe width of 10 nm, and 1383 had $x=0.10$ and a SiGe of 90 nm. The uncertainty in the Ge fraction of all samples is ±0.02. Photoluminescence (PL) spectra were measured using a Bomem DA8 Fourier transform infrared spectrometer (FTIR) and a room-temperature InGaAs detector. The excitation source was an Ar$^+$-ion laser emitting well above the band gap of silicon. Measurements were taken at 2 and 77 K. At 2 K, the as-grown samples exhibited sharp phonon-resolved bound exciton luminescence similar to that described in Refs. 5–7 [Fig. 1(a)].

The samples were then implanted with Si^{29+} ions at an accelerating voltage of 50 keV with no intentional heating or cooling of the substrates. The implants were performed by IICO of Santa Clara, CA, using an ion implanter regularly used for the commercial production of integrated circuits. The Si^{29+} isotope was chosen to prevent any mass interference with possible Fe^{56++} and N$_2^+$ ions in the ion implanter. The mass separation capability of the ion implanter beam line was maximized by adjusting the slits used for mass filtering

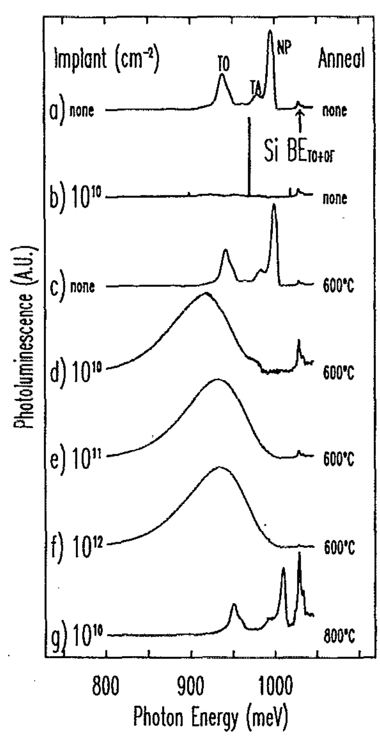

FIG. 1. 2 K photoluminescence spectra of sample 733 ($x=0.20$, ~6 nm (a) as grown, (b) after 10^{10} cm^{-2} 50 keV Si^{29+} implant, (c) after 10 min 600 °C anneal (no implant), (d) after 10^{10} cm^{-2} implant and 600 °C anneal (e) after 10^{11} cm^{-2} implant and 600 °C anneal, (f) after 10^{12} cm^{-2} implant and 600 °C anneal, and (g) after 10^{10} cm^{-2} implant and 800 °C anneal. In (g) the silicon photoluminescence was suppressed by a filter.

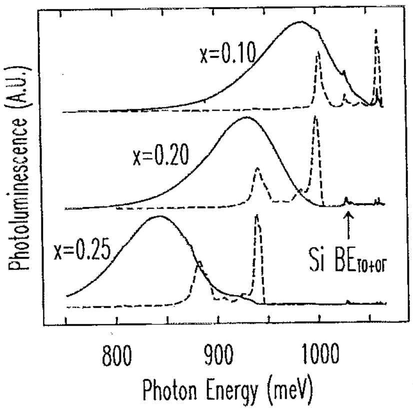

FIG. 2. 2 K photoluminescence of samples 1383, 733, and 746 (x=0.10 ±0.02, 0.20, 0.25, respectively) with 600 °C anneals both directly after growth (dashed lines) and after 10^{11} cm^{-2} 50 keV Si^{29+} ion implants (solid lines).

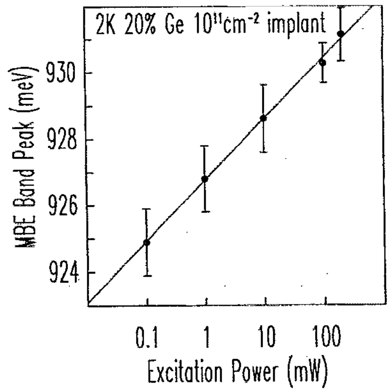

FIG. 3. Position of the peak of the deep luminescence in sample 733 (x =0.2, ~6 nm) after 10^{10} cm^{-2} Si^{29+} 50 keV implant and 600 °C annealing as a function of the pump laser power.

to an absolute minimum. When tuning the magnet current, the beam current at the peak of the Si^{29+} position (at which the implants were performed) was over forty times greater than that at the valley between the positions for Si^{28+} and Si^{29+}. The doses ranged from 10^{10} to 10^{12} cm^{-2}. After implantation, the samples were split into several pieces for further processing. The luminescence spectra of the samples without further processing were dominated by the Si substrate and a sharp line at 969 meV, and the phonon-resolved SiGe excitonic luminescence disappeared [see Fig. 1(b)]. The 969 meV signal may be the G-line associated with two carbon atoms in silicon, especially since a slight phonon replica separated from the main line by 72 meV was also seen.[14]

One series of samples was then annealed for 10 min at 600 °C. The furnace ambient was oxygen when the samples were loaded but was then immediately switched to nitrogen. After this step, all implanted samples showed a broad deep luminescence, with a peak 80–100 meV below the no-phonon (NP) bound exciton peak of the unimplanted samples. Figure 2 shows the results with implants of 10^{11} cm^{-2} (solid line) and no implant (simultaneously annealed, dashed line) for different Ge concentrations. The unimplanted $Si_{1-x}Ge_x$ annealed with the implanted samples showed the usual band-edge luminescence, so that the deep luminescence can clearly be attributed to an effect of the ion implant. Note that the corresponding deep luminescence seen in MBE SiGe is often not observed as grown, but similarly emerges after a moderate (e.g., 600 °C) anneal,[1] presumably due to the removal of nonradiative defects which sharply reduce the carrier lifetime. That the deep PL tracks the band-edge of the strained alloy layer shows that it originates from the $Si_{1-x}Ge_x$, and not from the Si layers. The full width half maximum (FWHM) of the deep PL is ~80 meV, again similar to the MBE results. Because of the similarity of the deep band in our results to that previously seen in samples grown by MBE, for the rest of this letter we refer to the deep band in our samples as the MBE band.

The dependence of this MBE band on implant dose, as seen in Fig. 1, was an increase in intensity (shown relative to the Si substrate bound exciton feature at 1030 meV) and a small upward energy shift with larger implant dose. Whether the energy shift is a real effect or due to some unintentional variation in the sample composition is not known. Another series of samples was annealed at 800 °C instead of 600 °C. Figure 1(g) shows the spectrum for the lowest implant sample. In this case, the MBE-band luminescence was not observed, and band-edge excitonic luminescence reappeared, although weaker than that in the original samples. The same behavior was seen in the samples with larger implant but the recovered excitonic luminescence was still lower in intensity. A similar behavior of a loss of strong broad PL and an emergence of band-edge phonon-resolved excitonic PL has been observed with annealing (700 °C) in the case of MBE.[2,15] It should be noted that in our experiments, the MBE-band luminescence was not observed in bulk silicon substrates which were implanted and annealed along with the $Si_{1-x}Ge_x$ samples. Furthermore, no luminescence was observed in the annealed $Si_{1-x}Ge_x$ samples which could be correlated with the Si regions of those samples (other than the Si band-edge exciton lines). This again, is similar to the MBE results, in that the broad band luminescence has not been observed for pure Si layers grown by MBE.

Finally, for the 10^{11} cm^{-2} implant in sample 733 (x =0.2), we show the dependence of the peak position of the MBE band (after 600 °C annealing) on the excitation power between 0.1 and 200 mW (Fig. 3). This dependence is similar to that reported for the same band in samples grown by MBE.[15] As a function of temperature, the peak shifted by about 30 meV to lower energy between 2 and 77 K. This is again consistent with the observation of a downward thermalization shift of about 45 meV between 10 and 80 K in MBE grown samples.[15]

The peak position of the deep luminescence in our experiments, its linewidth, annealing dependence, pump power dependence, temperature dependence, and dependences on the Ge fraction are all similar if not identical to the luminescence observed in samples grown by MBE. We therefore conclude that the center responsible for the deep broad PL in our samples is the same as that responsible for the corresponding PL in MBE samples.

As mentioned in the introduction, existing models for the MBE band include an optically active defect,[2] Ge-rich platelets,[9] and donor–acceptor pairs.[12] In our samples, the MBE band is observed for implanted Si doses as small as 10^{10} cm^{-2}, corresponding to a peak density of $\sim 10^{15}$ cm^{-3}, which implies an implantation of unintentional species many orders of magnitude lower. Because of this low density of implanted undesired impurities, and because of the annealing behavior, we conclude that donor–acceptor pairs are not responsible for the MBE band luminescence. Residual implantation damage of point defects, or defect clusters, are a plausible explanation of the MBE-band luminescence in our experiments and would easily explain the disappearance of the band with high-temperature annealing. Note that the damage introduced by silicon ion implants, even at low doses, are not isolated point defects but defect clusters related to the track of an implanted ion and recoiled atoms in the substrate.[16] Although less likely, it is also plausible that the defect clusters lead to the formation of the platelets often correlated with conventional MBE broad band luminescence, and that these platelets are the source of the luminescence. In either case, it appears that the presence of Ge atoms, or the presence of compressive strain, or both, is required for the MBE-band luminescence.

The formation mechanism for the centers responsible for the MBE band in MBE samples is not known. However, if one assumes a similar formation mechanism for the broad band PL centers in MBE samples and those in our experiment, one needs to identify a source of radiation damage in MBE. This might be the direct effect of stray electron radiation (from the evaporators) on the sample itself, or an indirect effect of ionization of a small fraction of the Si or Ge flux by the electron beams or other means (and subsequent acceleration) of the ions. Such mechanisms might indeed be expected to vary widely from chamber to chamber and explain differing results. A formation mechanism for the MBE-band center inherent to the low growth temperature MBE deposition process does not seem likely, however, as phonon-resolved excitonic PL without the deep band has been observed in some MBE samples grown as low as 300 °C.[4,11]

In summary, ion implantation and annealing has been used to switch the luminescence in $Si_{1-x}Ge_x$ quantum wells from a photon-resolved band-edge bound exciton process to a strong broad band well below the band edge, similar to that observed in some samples grown by MBE. The dependence of this deep luminescence on annealing, Ge fraction, pump power, and temperature are all similar to that observed in MBE samples. While a donor–acceptor pair transition mechanism is inconsistent with our results, the exact physical origin of the luminescence center is still not clear.

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