Characterization of $Si/Si_{1-x}Ge_x/Si$ quantum wells by cathodoluminescence imaging and spectroscopy

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Cathodoluminescence (CL) imaging and spectroscopy have been used to characterize fully strained SiGe quantum wells grown on Si. At $T\approx5$ K, the CL spectra contain only band edge luminescence features. Monochromatic imaging with the no-phonon line attributed to the bound excitons in the quantum well, has shown that the distribution of the luminescence from the wells is not uniform. The thinnest well (33 Å) contained a low density of nonradiative (luminescence reduction up to 100%) spots 40–100 μm in size. The thickest well (500 Å) contained similar nonradiative spots and also dark line features oriented along the ⟨110⟩ directions. These dark line features are areas of nonradiative recombination (up to 70%) and have been identified by transmission electron microscopy as misfit dislocations.

Strained $Si_{1-x}Ge_x$ alloy layers and SiGe quantum well (QW) structures grown on Si have become the subject of extensive research interest due to the possibility of improved device performance and capabilities. There is a specific interest for the optoelectronic industry in Si/SiGe heterojunction technology[1] with the potential for both Si-based optoelectronic detectors and emitters. Photoluminescence (PL) spectroscopy has been used to characterize strained Si/SiGe heterostructures[2] and QWs grown by molecular beam epitaxy (MBE).[3] Early MBE samples exhibited only very weak or broad luminescence features,[2,3] with excitonic features observed only for a thick layer with 4% Ge.[4] Recently, application of the first rapid thermal chemical vapor deposition (RTCVD)[5] and later improved MBE techniques[6] showed that high quality fully strained SiGe QWs could be grown which exhibited well-resolved luminescence of excitons. These recent advances have revitalized interest in the possibility of Si-based optoelectronic devices. Therefore a detailed analysis of the optical properties of such structures is required.

It has recently been demonstrated that cathodoluminescence (CL) imaging and spectroscopy can be applied to Si and SiGe for mapping luminescence features both laterally and in depth.[7] We report in this letter the first low temperature CL spectra containing well-resolved band edge luminescence and CL images from SiGe QWs.

CL spectra were recorded from both single (SQW) and multiple (MQW) quantum wells with different well widths grown by RTCVD on Si(100) substrates. In addition, CL measurements were made on SiGe/Si SWQs and MQWs grown by other variants of CVD growth for comparison; these results will be published elsewhere. In this letter we concentrate on the CL measurements recorded from two single strained $Si_{1-x}Ge_x$ samples grown by RTCVD. The samples consisted of a single strained epitaxial $Si_{1-x}Ge_x$ QW on a Si buffer layer (≈1 μm) with a thin ≈150 Å Si capping layer. Both samples had a germanium content of 20%, and well widths of 33 and 500 Å. These values were determined by high resolution transmission electron microscopy and Rutherford backscattering spectroscopy.[8] PL measurements have also been carried out on these samples at 4.2 K.

CL measurements were made at $T\approx5$ K using a JEOL JSM 35C scanning electron microscope fitted with an adjustable cold stage, a retractable off-axis paraboloidal collector mirror, and a grating monochromator (mono-CL, Oxford Instruments). The detector employed was a North Coast germanium diode detector. CL spectra were recorded using beam energies (E_0) from 10 to 35 keV with different beam currents (I_b) between 0.1 and 100 nA. The CL spectra were recorded with a spectral resolution of 2 nm.

CL spectra recorded from the 33 Å well sample and the 500 Å well sample are shown in Figs. 1(a) and 1(b), respectively. The spectral features are the same as the major features found in the PL spectra[8] although at much lower resolution. These are attributed to an exciton bound to a shallow impurity. The highest energy feature X_{NP} is associated with the no-phonon (NP) transition and the lower energy feature is associated with the Si-Si TO phonon-assisted transition. The TA phonon replica and Si-Ge and Ge-Ge TO features observed in the PL spectra cannot be resolved in the CL spectra.

On inspection of the CL spectra a shift of ≈49 meV is observed between the NP peaks in the two samples. This is quantitatively in good agreement with that expected by quantum confinement effects, with a blueshift of 45 meV from an infinitely wide well having been calculated for the 33 Å well.[9] The PL spectra recorded on the 500 Å sample showed wider linewidths compared with the 33 Å sample, whereas in the CL spectra the situation is reversed. These differences could be associated with the different carrier generation rates in the CL spectra and the PL spectra and local heating effects in the former. In addition, the luminescence intensity of the 500 Å sample was an order of magnitude weaker than the 33

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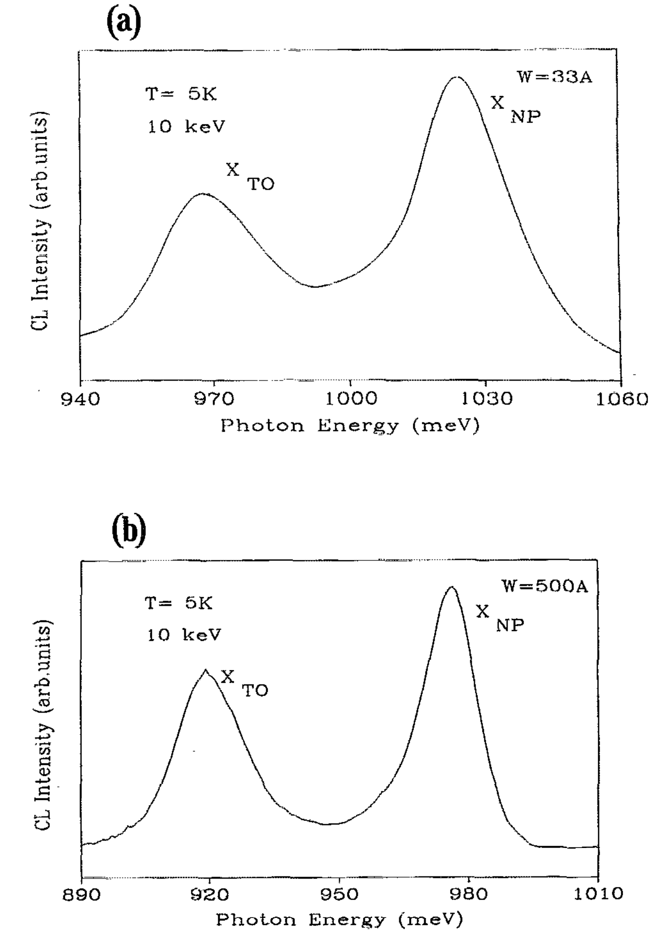

FIG. 1. CL spectra recorded at $T \approx 5$ K, $E_0 = 10$ keV, $I_b = 0.1$ nA: (a) QW $Si_{0.8}Ge_{0.2}$, thickness 33 Å, (b) QW $Si_{0.8}Ge_{0.2}$, thickness 500 Å.

Å sample, presumably due to the higher concentration of nonradiative centers.

CL imaging measurements were made using the X_{NP} feature. Figure 2(a) shows the CL image of the 33 Å well recorded at $T \approx 5$ K. On inspection of the image it is clear that the luminescence from the well is not uniform, and contains a low density of dark spots with dimensions between 30 and 100 μm. Monochromatic line scans showed that these dark spots are areas of nonradiative recombination with a luminescence reduction of up to 100%. Some areas show different levels of nonradiative recombination; the reduction in luminescence can vary from 65% to 100%. An estimate of the spatial resolution can be made assuming that the energy dissipation volume is a sphere of diameter equal to that determined by the Gruen range.[10] However, we have observed previously that in both bulk Si and SiGe alloys the CL spatial resolution can be greatly affected by the large exciton diffusion lengths. CL spectra recorded as a function of beam energy showed that bound exciton luminescence from the underlying Si substrate could only be observed at $E_0 \geqslant 15$ keV indicating negligible exciton diffusion at lower beam energies. The CL images were recorded at $E_0 = 10$ keV, and the spatial resolution was estimated to be of the order of 1 μm. Therefore the shape of these dark spots is not effected by the spatial resolution.

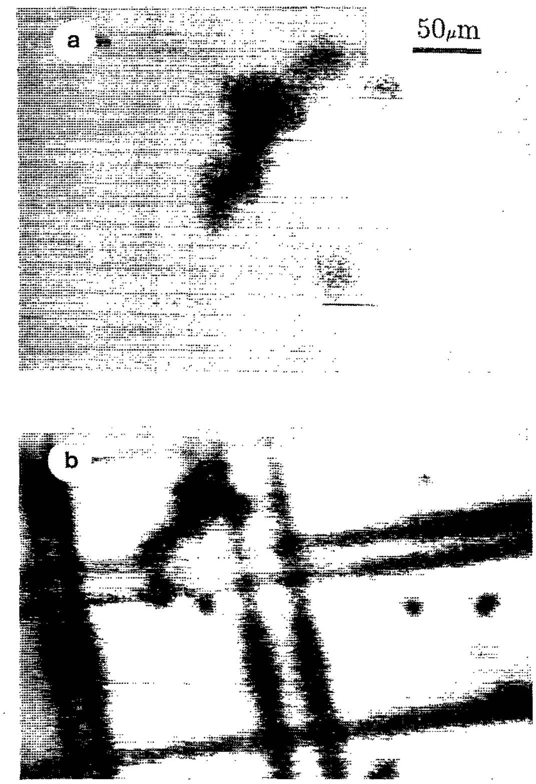

FIG. 2. Monochromatic CL images recorded at $T \approx 5$ K, $E_0 = 10$ keV, $I_b = 0.1$ nA: QW $Si_{0.8}Ge_{0.2}$, thickness 33 Å, (b) QW $Si_{0.8}Ge_{0.2}$, thickness 500 Å.

On inspection of the CL image of the 500 Å well [see Fig. 2(b)], similar dark spots can be seen together with dark lines oriented along the ⟨110⟩ directions. These dark line features are also areas of nonradiative recombination with a reduction in luminescence intensity of up to 70%. Similar CL dark line contrast has been observed in CL imaging experiments on Si/SiGe epilayers containing misfit dislocations.[11] Transmission electron microscopy (TEM) was used to examine the areas where the CL measurements were carried out to try and determine the source of the dark line features and the dark spots. A 1:1 correlation was established between the dark line contrast and the misfit dislocations. The misfit dislocations were all 60° type with Burgers vector $(a/2)\langle 110 \rangle$. However no unusual structural features could be correlated with the dark spots, suggesting that these areas of nonradiative recombination could be due to point defects trapped by the interfacial strain in the QW. The average density of these dark spots varied from 10^3 to 10^4 cm^{-2}, but densities as low as 10^2 cm^{-2} were observed in other SiGe samples grown in the same growth chamber. This dark-spot-type defect has been observed at higher densities in CL mapping of QWs grown by other CVD techniques and these results will be reported elsewhere.

Dislocation-related D-band luminescence has been observed in $Si_{1-x}Ge_x$ alloy layers grown on Si by liquid phase epitaxy[12] and other growth techniques. Although there are misfit dislocations present in the 500 Å QW sample no D bands were observed in either the CL or PL spectra. However, it has been demonstrated that D-band luminescence is not observed in the absence of transition metal

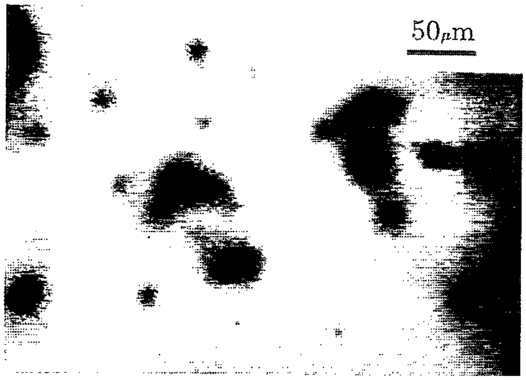

FIG. 3. Monochromatic CL image recorded of the SiGe 500 Å sample, after annealing for 1 h at T=300 °C.

contamination.[13] It has also been shown that low pressure CVD growth can produce Si epitaxial layers with very low levels of transition metal contamination.[14]

To investigate the stability of the nonradiative recombination centers, both the 33 and 500 Å well samples were annealed in the temperature range 100–400 °C. CL spectra and images were recorded from the samples before and after annealing. Each sample was cut into four sections, which were RCA cleaned and then annealed in flowing argon in a RCA cleaned quartz tube. Below 300 °C no differences were observed in the CL spectra or images. At 300 and 400 °C dramatic changes occurred in the CL images of the 500 Å sample. There were two distinct effects. First the dark spots became much larger; Fig. 3 shows the CL micrograph of a typical region. However, on closer inspection it was clear there were three distinct regions. In addition to the area of larger spots, there was a region with medium sized and small spots and a region where there were no spots observed. The second effect which occurred over the whole sample was that the dark line CL contrast at the misfit dislocations disappeared [compare Figs. 2(b) with Fig. 3]. However, TEM analysis revealed that the misfit dislocations were still in the sample and the nature of the misfit dislocations had not changed after annealing. CL spectra from the 500 Å QW sample showed a dramatic increase in the SiGe exciton peak intensity (increase by 30–50 times) following annealing at 300 and 400 °C. CL images from the annealed 33 Å well samples showed a small reduction in the density of dark spots on annealing at temperatures greater than 300 °C. In contrast with the 500 Å sample there was only a small increase (2–4 times increase) in the CL luminescence intensity, probably because there were fewer nonradiative recombination centers.

The annealing treatment of the 500 Å sample has increased the radiative recombination in the SiGe layer, and the CL images have shown that the nonradiative recombination at the dislocations is no longer observed even though the dislocations are still there. This suggests that the nonradiative recombination centers at the dislocations have either been destroyed or passivated. There have been well-documented case of hydrogen passivation of both deep and shallow levels in Si.[15] It is possible that the passivation could be caused by hydrogen incorporated during layer growth, and that the annealing step has redistributed it. It is difficult to tell if the average density of dark spots has changed on annealing, but in general there are more areas without any dark spots and dark line contrast. CL spectra were recorded in both regions. It was found that there was a reduction in CL intensity in the areas where the dark spots became larger, and an increase in the areas where there were no large dark spots. CL spectroscopy revealed that the overall sample luminescence had increased after annealing. This increase in luminescence intensity is caused by a reduction in the nonradiative centers in the material.

The annealing treatment effects are not so dramatic in the 33 Å well material due to the lower density of dark spots and because there are no areas of nonradiative recombination at the misfit dislocations. That is, there are only very few areas of nonradiative recombination and the annealing treatment has only a small effect on increasing the luminescence efficiency.

This study has demonstrated the feasibility of using CL to obtain spatial information about the luminescence features and nonradiative processes occurring in Si/SiGe QWs. Further work is necessary to identify the nonradiative centers responsible for the dark spots and the effects of annealing and the possible role of hydrogen.

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