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Photoluminescence from Si/Si_{0.87}Ge_{0.13} multiple quantum well wires

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Abstract: This paper reports a low temperature photoluminescence study of the optical properties of a series of dry etched free standing strained layer Si/Si_{0.87}Ge_{0.13} multiple quantum well wires with lateral dimensions between 40nm and 500nm. The results show that dry etching induces partial strain relaxation. An enhanced electron-hole droplets emission from the Si layers with reducing wire width was observed due to both the extra surface roughness introduced during the etching process, which accelerates the nucleation of the droplets formation, and the effect of lateral confinement. A new feature at 1.131eV at 4K related to unknown impurity states located at the heterointerfaces was also detected.

The optical properties of semiconductor nanostructures, such as quantum wires and dots fabricated by using different techniques, have been of world-wide interest^[1] recently due to their potential applications in device engineering. Si/Si_{1-x}Ge_x heterostructures, as one of the recently emerged new materials, have also been widely investigated^[2-5] with most of the emphasis on optical properties of quasi-two dimensional (2D) structures. With the application of electron beam lithography and reactive ion etching, nanostructures have been successfully fabricated in modulation doped p⁺-Si/Si_{1-x}Ge_x heterojunctions with feature size down to 15nm.^[6,7] Due to the extremely low sidewall damage inflicted during dry etching of Si/Si_{1-x}Ge_x system as compared to GaAs/Al_{1-x}Ga_xAs system,^[8] the study of the physical properties of Si/Si_{1-x}Ge_x nanostructures is most promising. Our previous studies on the optical properties of nanostructured wires based on a modulation doped p⁺-Si/SiGe 2D hole gas indicate that a strain relaxation process occurs during the wire fabrication and a blue shift of quantum confined transitions with reducing lateral dimension down to below about 40nm can be observed.^[6,7] In this paper, we report a study on the photoluminescence (PL) of a series of Si/Si_{1-x}Ge_x multiple quantum well (MQW) wires. In addition to the features similar to

those reported on the 2D hole gas wires, an enhanced electron-hole droplet (EHD) emission and a new feature related to impurity states at the Si/Si_{1-x}Ge_x heterointerfaces have been observed in the MQW wires.

The original material was grown by molecular beam epitaxy (MBE) on a (100) oriented n-Si ($\rho \sim 20\Omega\text{-cm}$) substrate. The MBE sample has 30 periods of Si/Si_{0.87}Ge_{0.13} MQWs with the well and barrier widths of 8nm and 21nm, respectively, grown on a 200nm Si buffer layer. They were first scribed into a series of 5mm x 5mm chips, and then cleaned and patterned with wires of different sizes by using electron beam lithography and lift-off of the resist.

The reactive ion etching was performed on a planar reaction chamber system operated at an rf frequency of 13.56MHz. The etching gas was 99.99% pure SiCl₄. By using optimized etching parameters, i.e. an rf power of 35W, a gas flow rate of 2.25sccm, and a chamber pressure of 10.8mTorr, which gives an etching rate of 25nm/min, we obtained a series of 2.5 μm long wires with their widths between 40nm and 500nm and pitch size of 750nm. The etched depth was kept to about 0.6 μm , i.e. half of the MQW layers was cut into wires, so that signals from both the wires and the remaining MQWs could be observed simultaneously, and the latter serves as a control sample in the experiments.

The PL spectra were measured at temperatures between 4K and 20K on a standard cryostat system, using the 488nm line of an Ar⁺ ion laser with a power density variable between 0.1 and 50W/cm². The PL signal was detected by a liquid N₂ cooled Ge detector through a Jobin-Yvon THR1000 monochromator.

Fig.1 shows the PL spectra of a MQW sample (curve b) and four wire samples (curves c-f) at 4K. For comparison, a PL spectrum from a deep etched sample (curve a) is also plotted in Fig.1, from which all the epitaxially grown layers were removed. The PL spectra were obtained by illuminating a constant area on samples with different lateral sizes, i.e. less MQW areas were exposed to the laser beam during the measurements with reducing wire width. It can be seen that peaks 1 and 4 are from the substrate, which are the bound exciton no-phonon line (BE_{Si}) and the TO phonon assisted bound exciton (BE^{TO}_{Si}) line,^[2,3] respectively; peaks 3 and 5 are TO phonon assisted free exciton (FE^{TO}_{Si}) line and the EHD emission is related to the Si buffer layer or the Si layers in the MQWs, which is about 12meV below the BE^{TO}_{Si} line. It is clear that even with less illuminated areas on the wires, an enhanced luminescence of EHD with reducing wire width is observed under the same excitation condition. This is possibly due to the wire confinement and/or the increasing surface roughness^[9,10] introduced during the wire fabrication process, which improves the formation of the nucleation of the droplets, leading to stronger PL in the experiments. In addition to the peaks discussed above, other excitonic features (peaks 6-8) related to the SiGe layers in the MQWs are also observed, which are no-phonon and TO phonon assisted PL lines. The low energy broad band transition (band 9) at ~0.8eV existing in both the MQWs and a 500nm wide wire sample might be related to strain or dislocations, and a new feature X_I (peak 2) located between the no-phonon and TO phonon assisted Si PL lines emerges in both the MQWs and the wire samples. Peak 2 is from the Si buffer layer or the Si layers in the MQWs due to its energy position. When the wire width is reduced to about 200nm, the broad band 9 disappears, a new defect-related peak (peak 10) emerges at 0.76eV and the peaks related to the SiGe layers (peaks 6, 7) split into two. The splitting suggests that strain relaxation occurred during dry etching. While the splitting of peak 2 suggests that it comes from the Si layers in the MQWs due to that only half of the MQWs was etched

away, no double structure should be seen if it were from the Si buffer layer. The blue shift of the split peak is due to strain relaxation in the Si layers as half of the MQWs was etched away.

Fig.1 PL spectra of different samples at 4K. The excitation power was $10\text{W}/\text{cm}^2$. The peaks are marked by numbers: (1): BE_{Si} ; (2): X_{I} ; (3): $\text{FET}^{\text{TO}}_{\text{Si}}$; (4): $\text{BE}^{\text{TO}}_{\text{Si}}$; (5): EHD; (6): $\text{XNP}_{\text{Si-Ge}}$; (7): SiGe related; (8): $\text{XT}^{\text{TO}}_{\text{Si-Ge}}$; (9): strain related; (10): defects. (a) deep etched sample; (b) multiple quantum wells; (c) $2.5\mu\text{m} \times 500\text{nm}$ wires; (d) $2.5\mu\text{m} \times 200\text{nm}$ wires; (e) $2.5\mu\text{m} \times 100\text{nm}$ wires; (f) $2.5\mu\text{m} \times 40\text{nm}$ wires.

Fig.2 Line shape fitting of the EHD emission from two samples. The solid lines are experimental PL spectra at 4K, and the dashed lines are least square fittings to the EHD emissions. The arrows marked the positions of μ and $E'_g - \hbar\Omega$, where $\hbar\Omega$ is the TO phonon energy. (a) $2.5\mu\text{m} \times 500\text{nm}$ wires; (b) $2.5\mu\text{m} \times 40\text{nm}$ wires.

Fig. 2 show an example of line shape analysis on the EHD emission observed in Fig.1. Spectrum *a* is from the 500nm wires and spectrum *b* from the 40nm wires. Parameters such as E'_g , the renormalized band gap energy, the chemical potential μ , and

the electron-hole pair density in the droplets n . are obtained By comparing the results from spectra taken at both low and high optical pumping powers, the EHD binding energies from different samples under different experimental conditions can be estimated.^[9] One can find that with decreasing lateral size from 500nm to 40nm, the EHD binding energy changes from 11.3meV to 13.6meV, and the electron-hole pair density increases indicating an increase in the radius of the EHD in confined system.

The origin of band 9 in Fig.1 needs more investigation, but a possible explanation for the intensity drop and disappearance of it with reducing wire width is that this band may come from strain in the epitaxial layers. As half of the MQWs was etched into wide wires, the strain will be partially relaxed, causing a decrease in its PL intensity. As the wires narrow further, more dry etching damaged areas are probed in the experiments. Although half of the MQWs remains untouched, the surface damage and the total relaxation of strain in the MQW wires may extinguish the PL signal (band 9) from the samples.

Through detailed study of the behavior of the new feature X_I ,^[11] we have identified it as an impurity related emission. With the increase of temperature, the PL intensity of X_I gradually drops to zero compared to the intrinsic PL emission $X_{NP-Si-Ge}$. At a certain temperature, the PL intensity of X_I saturates with the increase of the optical pumping power. These properties indicate that X_I is a transition related to impurities. We propose that X_I arises from impurity states of unknown origin located at or in Si layers close to the heterointerfaces. The feature in low temperature PL spectra may be from an unidentified impurity-to-band transition as it was also observable in photoreflectance measurements.^[11]

In conclusion, we have investigated the photoluminescence of dry etched free standing Si/Si_{1-x}Ge_x MQW wires. The results show that in addition to the luminescence due to a strain relaxation process arising from the etching, an enhanced emission from EHD in the wires with reduced lateral dimension and a new feature probably due to impurity states located at the Si/SiGe heterointerfaces are also observed.

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