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Growth Criteria for Establishing Luminescence in Strained $Si_{1-x}Ge_x/Si$ Quantum Wells

S.Fukatsu, H.Sunamura, Y.Kato, N.Usami, and Y.Shiraki
Research Center for Advanced Science and Technology (RCAST), The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153, Japan

Successful and reproducible growth of strained quantum wells (QWs) is demonstrated, addressing the selection of higher growth temperature as a criterion to establish a high degree of structural integrity with maintaining a good crystallinity in terms of "optical" quality. The temperature threshold was found to be correlated with luminescence efficiency while the threshold was different for the crystal orientation. Ge-rich layers, x>0.35, were grown, in which well phonon-resolved luminescence was obtained. Growth and PL of QWs on vicinal surface are demonstrated.

I. Introduction

Recent advance in Si epitaxial technology has accelerated the research on luminescence properties in SiGe-based heterostructural systems. First study was reported by Sturm *et al.* on exciton luminescence in strained $Si_{1-x}Ge_x/Si$ quantum wells (QW) grown using rapid thermal chemical vapor deposition[1]. Recently it was addressed that luminescence in QWs grown by solid source molecular beam epitaxy could be obtained only when one brings the growth temperature higher than a practical threshold, 620°C[2,3]. In contrast, it seems that the growth criterion to establish luminescence in gas source related growth methods has not been established. It has been rather postulated that the gas source grown QWs are of a high optical quality from its birth[1,4-7]. In this paper, we present an investigation on strained $Si_{1-x}Ge_x/Si$ QWs growth by gas source Si molecular beam epitaxy, and attempt to establish criteria to obtain efficient luminescence.

II. Experimental

Samples were grown by a purpose-built gas source Si molecular beam epitaxy (MBE) (Daido Hoxan VCE-S2020) on nominally on-axis Si substrates using Si_2H_6 and GeH_4 on Si substrates[7]. Growth temperature (Ts) was monitored by a thermocouple. Ge composition and layer thickness were determined by double crystal x-ray diffraction. Photoluminescence (PL) was recorded in standard lock-in configuration using an argon ion laser operating at an optical excitation density of 0.1-1W/cm^{-2} on the sample surface, a 1-m dispersive monochromator, and a liquid-nitrogen-cooled Ge detector. Sample temperature was controlled by a closed cycle refrigerator (>16K) or by immersion in pumped helium (≈2K).

III. Results and discussion

Emissivity of solid source MBE-grown $Si_{1-x}Ge_x$ QWs was found to depend critically on the growth temperature as has been revealed by previous studies[2,3]. This can be interpreted in terms of crystal quality, and correlated with post-growth annealing where band-edge luminescence was found to develop in less emissive QWs[8]. In contrast, a high degree of PL emissivity has been postulated to be inherent to gas source grown QWs[1,4-7]. In view of the annealing experiments having been done on solid source MBE grown QWs, the importance of crystal quality to the emissivity of QWs seems to be obvious. Hence, it is likely that PL efficiency depends on Ts also in gas source grown QWs.

Figure 1 shows 18K PL spectra of $Si_{1-x}Ge_x/Si$ SQWs of nominally same composition, x=0.18, and well width, Lz=34Å, grown on p-type Si(100) substrates at various temperatures. Phonon-resolved PL is observed between 950-1050meV. NP, TA, TO refer to no-phonon, transverse acoustic, and optical phonon replicas, respectively. Si^{TO} doublet peaks consists of free exciton line at the higher energy side and B-bound exciton line on the lower energy.

Obviously, QW PL intensity is seen to monotonically increase with Ts, and the integrated PL intensity is larger for QW compared to Si for Ts>700°C. Figure 2 shows the integrated intensity of QW luminescence as a function of Ts. For Ts>700°C, net intensity levels out and rapid PL quenching is evident with decreasing temperature, Ts<700°C.

All these findings are in qualitative agreement with the trend observed in solid source MBE grown QWs[2,3]. Alternatively, QW PL efficiency depends critically on growth temperature even in gas source MBE, and a higher Ts brings an improvement in QW PL intensity. To strengthen this idea, excitation

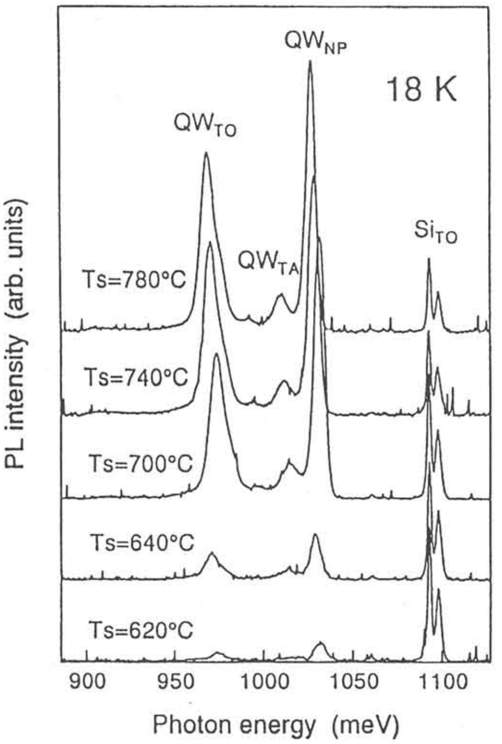

FIG.1. 18-K PL spectra of strained $Si_{1-x}Ge_x$/Si SQWs with x=0.18 and Lz=34Å grown by gas source MBE at various growth temperatures, Ts=620-780°C.

profile of PL intensity was studied[8]. Figure 3 shows the integrated intensity of four QWs grown at different temperatures as a function of excitation power. The absolute intensity for a fixed power increases with Ts as was already shown in Fig1. However, under intensive photopump, QW PL intensity seems to be of comparable magnitude, with the least emissive one (Ts=620°C) is catching up with others in intensity in the high excitation limit. Meanwhile, for lower excitation, intensity difference becomes noticeable. Such a trend can be visualized by looking at the power exponent, m, of excitation profile[8]. For comparison, m=1 line has been drawn aside. m=1 is indicative of radiative recombination rate directly proportional to the incident power, and the absence of nonradiative channels which would kill the number of available carriers. m<1 is expected for band filling, i.e. high excitation, and m≈2 indicates strong influence of nonradiative pathways, viz., carrier loss. Details of m is given Ref.8. Judging from these criteria, m<1 for higher excitation suggests effective reduction in the influence of nonradiative channels on PL efficiency.

Post-annealing was performed on gas source MBE-grown QWs[3,8,9]. Approximately two-fold increase was observed in PL intensity of QWs grown at Ts=620°C, whereas intensity increase was smaller for QWs when grown at Ts>700°C. It is noteworthy that E^{NP} exhibited significant upshift after annealing due to Ge/Si interdiffusion giving rise to a modulated potential[9]. However, no dislocation features were found in PL spectra, showing unmatched structural stability of QWs compared with rather thicker alloy layers[10]. Excitation profile of PL

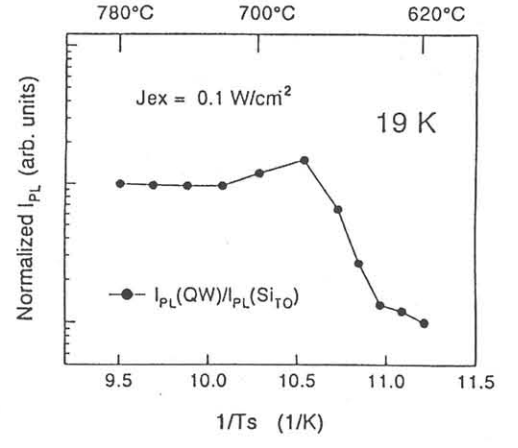

FIG.2. PL intensity of QW normalized to Si substrate PL as a function of Ts.

intensity after annealing exhibited qualitative change both in gas and solid source MBE-grown QWs. m increased following anneal, tending toward m=1 with concomitant increase in absolute intensity[8,10].

As seen from the foregoing discussion, it turns out that the quality of crystal is the key to establishing high PL efficiency regardless of growth schemes, be it gas source or solid source ones.

Figure 4 shows 2-K PL spectrum of a $Si_{0.823}Ge_{0.177}$/Si single quantum well (SQW) with well width (Lz) of 68Å grown at Ts=740°C in the good epitaxial temperature range addressed above. Highest energy line with a linewidth of 4meV is no-phonon line arising from alloy disordering. TO phonon lines are resolved into three lines corresponding to different bond arrangement[1]. TA line is seen between NP and TO lines. Si substrate luminescence looks relatively stronger than at 18K. This seems to be related with nonradiative recombination in the Si layers[7,8]. Integrated intensity

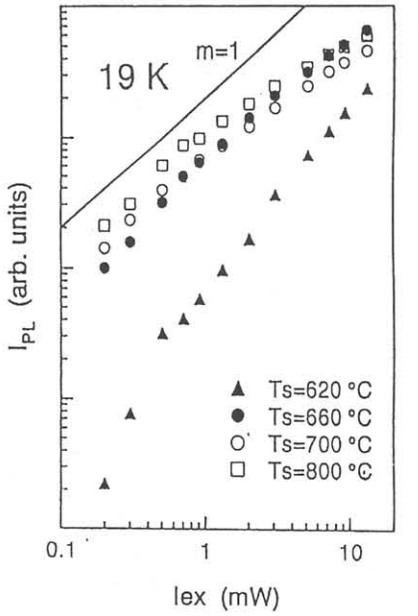

FIG.3. Excitation power dependence of PL intensity of QW. Solid line represents the power exponent m=1.

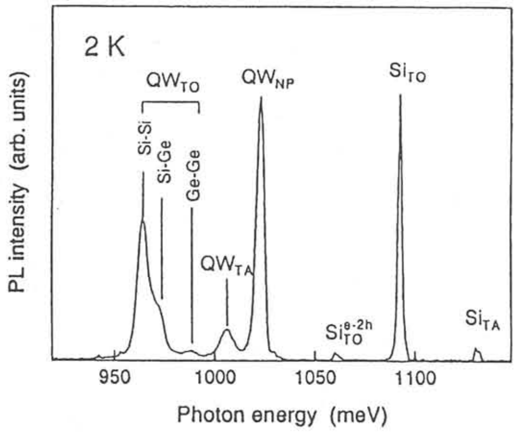

FIG.4. 2-K PL spectra of a strained $Si_{0.823}Ge_{0.177}/Si$ SQW.

of QW PL is, however, larger by an order of magnitude than that of Si PL. Note, all these lines are due to bound excitonic transitions. Seen at the lower energy side of Si^{TO} line is electron-2 hole pair luminescence located at 1155meV. At 1030meV, though superposed on QW PL, a small shoulder is seen, which is due to two-phonon involving transition, TO+O^{Γ} line. This is contrasted with previous PL spectra of QW PL grown by solid source MBE where Si dominated the spectra at 2K[11].

Growth of Ge rich QWs were performed for x> 0.31[12]. Figure 5 shows 16K PL spectra of QWs of x=0.31, 0.38, 0.47, and 0.57. Note, well width are not the same. Nevertheless, NP peak energy is seen to decrease with increasing x due to rapid increase of valence band confinement barriers with x. Second peak in each figure can be attributed to TO phonon replica of NP lines, as identified from peak separation, 57-59meV.

Finally, QW growth on vicinal surface is demonstrated in Fig.6 with PL spectra of QWs growth on on-axis wafer and vicinal surfaces, 3 and 4°-off misaligned toward [110], in the identical growth conditions. Spectral features are the same but there is a finite peak downshift for vicinal surface QWs. Details are not clarified yet.The surface

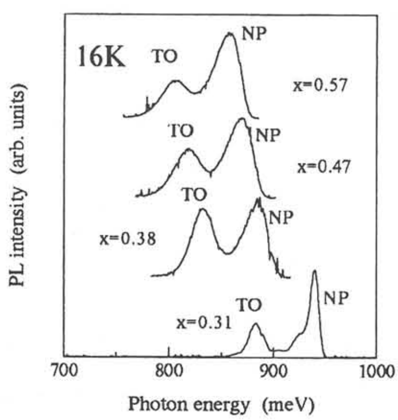

FIG.5. 16-K PL spectra of strained $Si_{1-x}Ge_x/Si$ SQW with x=0.31, 0.38, 0.47. 0.57.

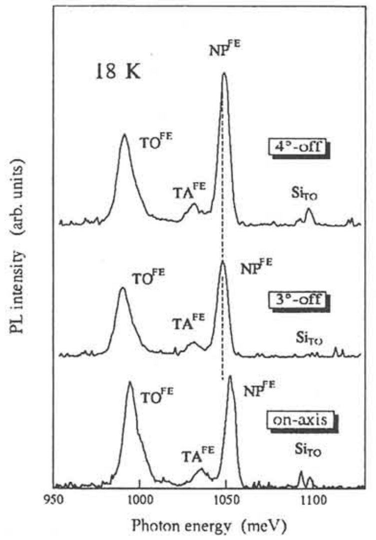

FIG.6. 16-K PL spectra of strained $Si_{1-x}Ge_x/Si$ SQWs (x=0.177, Lz=34Å) grownon on-axis (top) and vicinal surfaces; 3° and 4°-off toward [110].

morphology of 3 and 4°off substrates were almost featureless and smooth, providing a good quality of surface flatness.

IV. Conclusions

We presented a study on the growth of strained $Si_{1-x}Ge_x/Si$ quantum wells by monitoring photoluminescence emissivity as control. Selection of high growth temperature and post growth annealing were found to provide sufficient emissivity in otherwise scarcely emissive QWs. Ge rich QWs and vicinal surface QWs have been successfully grown.

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