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Excitonic Band Edge Luminescence in Strained $Si_{1-x}Ge_x$/Si Quantum Well Structures Grown by Gas-Source Si Molecular Beam Epitaxy

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Excitonic photoluminescence was observed from strained SiGe/Si quantum wells (QW) grown by gas source Si molecular beam epitaxy (GS-Si MBE). The well width dependence of PL emission energy was in good agreement with a square potential profile, showing that the "abrupt" Si/SiGe is created by GS-Si MBE. Photopump and transport of carriers characteristic of indirect gap materials was found. The majority of carriers are generated deep inside the substrate and subsequently transported to the quantum wells on the surface side.

I.Introduction

Since the first demonstration of band-edge photoluminescence (PL) by Sturm *et al.*[1], PL from strained SiGe/Si quantum well (QW) has attracted much interest recently[1-14]. In this paper, we investigated the quantum size effect and the carrier photogeneration and transport in strained SiGe/Si QWs. The latters are of importance since they may dictate the efficiency of PL and appropriate sample design taking into account the actual carrier delivery is desirable for efficient and controlled PL.

II.Experimental

Samples were grown on nominally on-axis Si(100) wafers by a purpose-built gas source Si molecular beam epitaxy[5,6,11] (GS-Si MBE) (Daido Sanso VCE-S2020) at 600-750°C using Si_2H_6 and GeH_4. Ge content, x=0.16, was determined for multiple QWs (MQWs) by x-ray diffraction. No misfit dislocations were found in cross-sectional transmission electron microscopy, showing the high quality of the samples. PL measurements were performed using an argon ion laser operating at an optical power of 0.25-30mW. Signals were recorded by a standard lock-in detection system using a 1-m monochromator and a liquid-nitrogen-cooled Ge detector. Sample temperature was controlled by immersion in liquid helium, or by a closed-cycle refeigerator.

III.Results and discussion

1. PL spectra and quantum confinement

Figure 1 shows a 18K excitonic band-edge PL spectrum of a $Si_{0.84}Ge_{0.16}$/Si (Lz=55Å) MQW. Luminescence lines labeled NP, TA and TO are attributed to no-phonon, transverse-acoustic- (TA) and TO-phonon-assisted emissions, respectively. NP line develops through momemtum-conserving scattering due to compositional alloy disordering. The energy difference of 58meV between NP and TO lines matches the TO phonon energy of Si. The other TO phonon features due to Si-Ge and Ge-Ge bondings in between TA and TO_{Si-Si} emission lines are well-resolved. Since the SiGe layer is under a compressive biaxial stress, a SiGe quantum well of type-I band alignment consisting of Δ_4 minima and heavy hole states is established between the Si barriers, where the conduction and valence band discontinuities are 10 and 136meV, respectively. The electron effective mass and heavy hole masses were assumed to be $0.19m_0$ and $0.278m_0$ throughout this study. Interestingly, the quantum confinement is essentially determined by the hole trapping since the electron confinement is so loose.

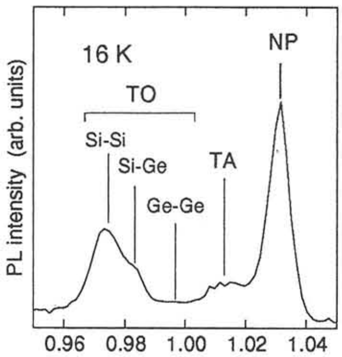

Fig.1. 18K PL spectra of a MQW with well widths of Lz=55Å.

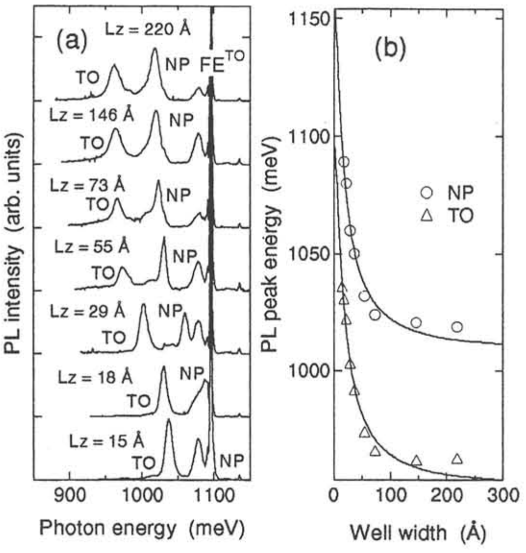

Fig.2. PL spectra of MQWs with different well widths and well width dependence of PL peak energies in MQWs.

PL spectra of $Si_{0.84}Ge_{0.16}/Si$ MQWs of different well widths are shown in Fig.2(a). It is seen that the PL emission energies systematically shift to higher energies with decreasing well width[6-11], i.e. quantum size effect is observed. Figure 2(b) shows the PL energy-shift vs well width where circles and triangles represent NP and TO peak energies, respectively. The solid lines represent the transition energies calculated with a square potential profile assuming an exciton binding energy of 15meV[7-10]. TO line energy is obtained by subtracting 58meV from the NP energy. The close agreement between the data and the calculation shows that an abrupt Si/SiGe interface can be created by GS-Si MBE. This is in sharp contrast with solid source MBE-grown QWs where the Ge segregation-induced potential profile distortion was found to shift the PL peak energies higher than the theoretical prediction.

Another interesting feature of Fig.2(a) is that the relative intensity of NP and TO lines is reverted around Lz=30Å which is comparable with the exciton Bohr radius ≈40Å. For thinner wells, TO lines dominate the spectra. This shows that the wavefunction of confined excitons penetrate into Si barriers and the alloy scattering is reduced.

2. Temperature dependence of PL

Spectral variation of PL with temperature for a 73Å-SQW[9] is shown in Fig.3. It is seen that SiGe QW emission is observed above 100K in contrast to a relatively rapid decay of Si emission for 30-50K. This supports the assumption of type-I QW formation. QW emissions begin to decrease above 80K with an activation energy of 130meV, reflecting the cofinement potential calculated by the theory[9].

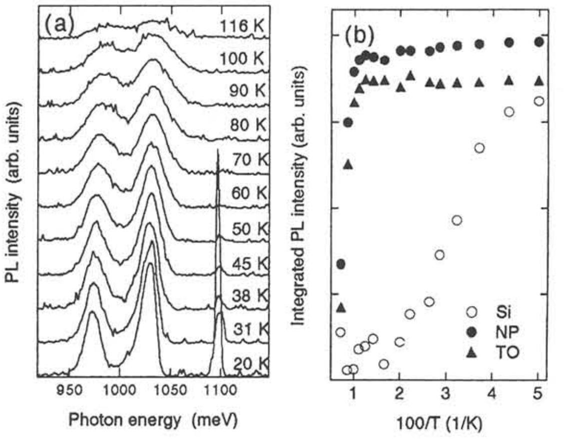

Fig.3. Temperature dependence of PL profile and integrated intensity of a SQW (Lz=73Å).

3. Carrier transport

Tempearture dependecne of PL spectra of a MQW with well widths of Lz=24,31,48Å is shown in Fig.4. The 24Å-well was grown first, followed by 31Å- and 48Å-wells. It is noted that PL of the 24Å-well located on the substrate side is the strongedst in intensity. The 24Å-well emission rapidly declines with increasing temperature whereas 31-Å and 48Å-well emissions begin to dominate the spectrum above 76K though the net emission intensity is gradually decreased. This behavior is related to the photon absorption process. Since Si has an absorption coefficient $10^3 cm^{-1}$ for a wavelength of 488-514.5nm and grown film thickness is not larger than 300nm, incident photons will penetrate into the Si substrate. Most of photocarriers, 99.7% or more, are created in the Si substrate and are then transported toward the quantum wells. Carrier transport diagram is schematically shown in Fig.5. Obviously, traveling carriers find the QW 1 on the substrate side first. At

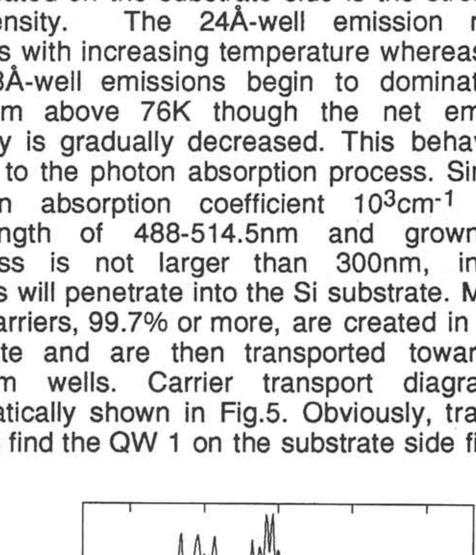

Fig.4. PL profile evolution with temperature of a MQW with well widths of Lz=24,31,48Å.

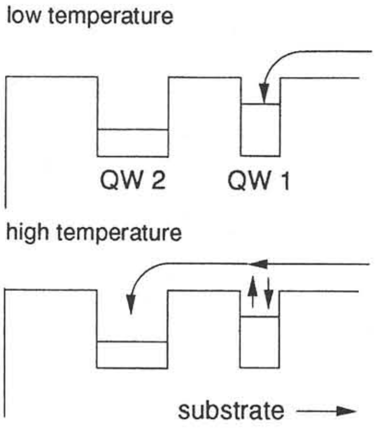

Fig.5. Photopump and subsequent carrier transport in a SiGe/Si MQW system.

sufficiently higher temperatures, carriers are no longer confined in the QW 1. Migrating carriers will then pass by the QW 1 and reach the QW 2. This is consistent with the temperature dependence of PL profiles in Fig.4 where 31Å- and 48Å-well emissions take over the PL spectrum above 60K. The present finding is likely to provide a fundamental aspect of photocarrier generation in indirect gap materials with small absorption coefficient.

IV.Conclusions

In summary, excitonic band-edge luminscence from strained SiGe/Si QWs and the quantum size effect was reported. Photocarriers were found to be created inside the Si substrate and subsequently transported to the QW wells. Present result is expected to hold a greater promise for the controlled optics with Si-based quantum confined structures.

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