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"Solid Source" Molecular Beam Epitaxial Growth of Highly Luminescent $Si_{1-x}Ge_x/Si$ Quantum Well Structures

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Highly luminescent $Si_{1-x}Ge_x/Si$ single quantum well (SQW) structures were successfully grown by conventional solid source Si molecular beam epitaxy adopting high growth temperature, Ts > 600°C. No-phonon (NP) transitions due to symmetry-breaking alloy disordering in SiGe layers and transverse optical (TO) phonon replicas were clearly identified. Well width dependence of transition energy was satisfactorily explained by theoretical calculation taking Ge surface segregation during growth into account. Excellent crystal quality was evidenced by total absence of defect-related deep level emissions characteristic of PL spectra of samples grown at lower temperatures. Present result indicates that high growth temperature environment is essential to efficient radiative recombination in SiGe/Si QW structures.

1. Introduction

In the field of optoelectronics, Si has not been recognized as a promising candidate for light emitting material because of poor recombination probability due to its inherent indirect nature of band structure. However, photoluminescence (PL) from SiGe/Si quantum wells (QWs) has recently provided a possibility to realize Si-based optoelectronic integrated circuits using Si processing techniques. Although there have been several reports of band edge emission from QWs using various techniques[1)-3)], no reports demonstrating strong band edge emission and quantum confinement in $Si_{1-x}Ge_x/Si$ QWs grown by conventional solid-source molecular beam epitaxy (MBE) have been made in spite of many efforts.

It has been said that low temperature growth at 400-600°C is effective to fabricate SiGe/Si strained layer growth. This is true when the width of a SiGe layer is close to the critical layer thickness predicted by equilibrium force balance theory. However, low temperature growth may cause poor quality of crystallinity with non-radiative pathways because of hampering surface migration of adatoms kinetically. This might be the reason why highly efficient luminescence has not been obtained so far in SiGe/Si QW structures grown by solid source Si MBE.

This paper describes the first successful "solid-source" MBE growth of highly luminescent $Si_{0.8}Ge_{0.2}/Si$ SQW structures. Our growth procedure makes no difference with the conventional method except selecting high growth temperature, Ts>600°C, beyond the conventional temperature window used for strained layer growth to date. Intense band edge luminescence of quantized states in $Si_{0.8}Ge_{0.2}/Si$ SQW was observed for the first time in MBE-grown samples. Systematic blue shift of PL lines was also clearly observed with decreasing well width. Theoretical calculation taking Ge surface segregation during growth into consideration explained this well width dependence. Systematic PL study of SiGe/Si SQW sturctures with well width of 30Å fabricated at different growth temperature ensured our idea that the crystallinity is essential to the efficient luminescence.

2. Experimental

The substrates were nominally on-axis p-type Si(100) wafers. All the samples were grown in a conventional MBE system (VG Semicon V80M). Si was evaporated from an e-gun and the beam flux was monitored by a quartz crystal oscillator. Ge was evaporated from an effusion cell. Ge content was determined from nominal growth rate and independently measured by double crystal x-ray diffraction of thicker alloy layers grown under identical conditions. Growth temperature was selected to be 620°C as measured by a thermocouple placed close behind the sample. Strain relief is unlikely at this temperature for thin SiGe well layers (10-100Å) with Ge content of 0.2 since the equilibrium critical thickness for this composition is predicted to be ≈120Å by Matthews and Blakeslee. In fact, no defect-related emissions characteristic to strain-relieved SiGe layers were observed in any of samples studied. PL spectra were recorded in a standard lock-in configuration and detected by Ge photodetector.

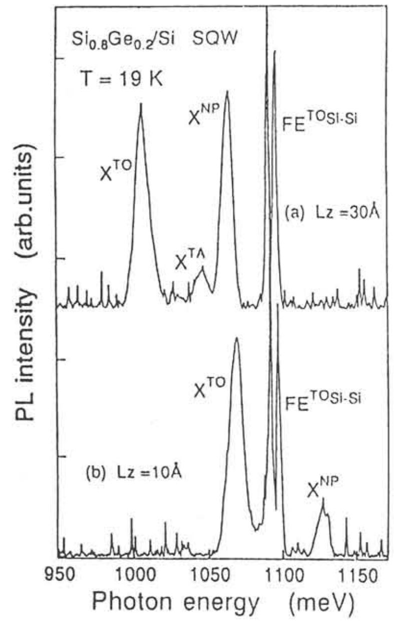

FIG.1. PL spectra of MBE-grown $Si_{0.8}Ge_{0.2}/Si$ SQWs.

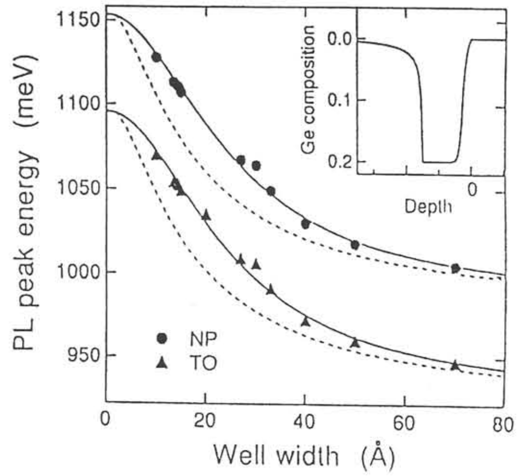

FIG.2. PL peak energy vs well width.

3. Results and Discussions

Figure 1 shows PL spectra of two $Si_{0.8}Ge_{0.2}/Si$ SQW structures grown at 620°C with well width (Lz) of (a)30Å and (b) 10Å, respectively. In addition to an intense line around 1094meV originating from radiative recombinations of excitons in the Si substrate, we can observe two sharp lines on the lower energy side. NP can be attributed to transitions with no phonon assistance in SiGe well layer due to symmetry-breaking alloy disorder, and TO is its phonon replica. The full width at half maximum of these lines is about 8meV which is comparable to the reported best value. The energy separation between TO and NP lines, 58mev, is consistent with TO phonon energy (Si-Si) in bulk Si. NP intensity reduction compared to TO for (b) is due to weakened alloy disorder because of wavefunction penetration into Si barrier layers .

The well width dependence of PL peaks in SiGe SQWs is shown in Fig.2. With decreasing well width, the emission energy is systematically blue-shifted. However, the peak energies are up-shifted by 10-30meV for Lz<40Å above the emission energy calculated assuming a square potential with a fixed exciton binding energy of 15meV (broken lines). It is known that the Si/Ge interface is smeared due to Ge surface segregation during MBE growth. Hence, the potential profile may not be a regular square but is skew-extended toward the surface like the inset of Fig.2. As shown in Fig.3, sputter depth profiles of SiGe QWs grown by two independent methods clearly shows Ge atoms segregate toward surface in the case of solid source Si MBE, whereas relatively sharp Si/SiGe interface is obtained by gas source MBE. The comprehensive treatment of the surface segregation of Ge atoms during Si MBE taking into account the alloy-specific effect of "self-limitation" associated with the atom site swap was first addressed by Fukatsu *et al.*[4] This scheme contains the atomistic arrangement and individual atom swap between the surface and subsurface sites. Solid line in Fig.2 is the result of precise calculation of excitonic transition energy taking the segregation profile of Ge atoms into account. Quantized bound states were numerically obtained by solving Schrödinger's equations for the potential profile divided into regions in units of atomic layer.

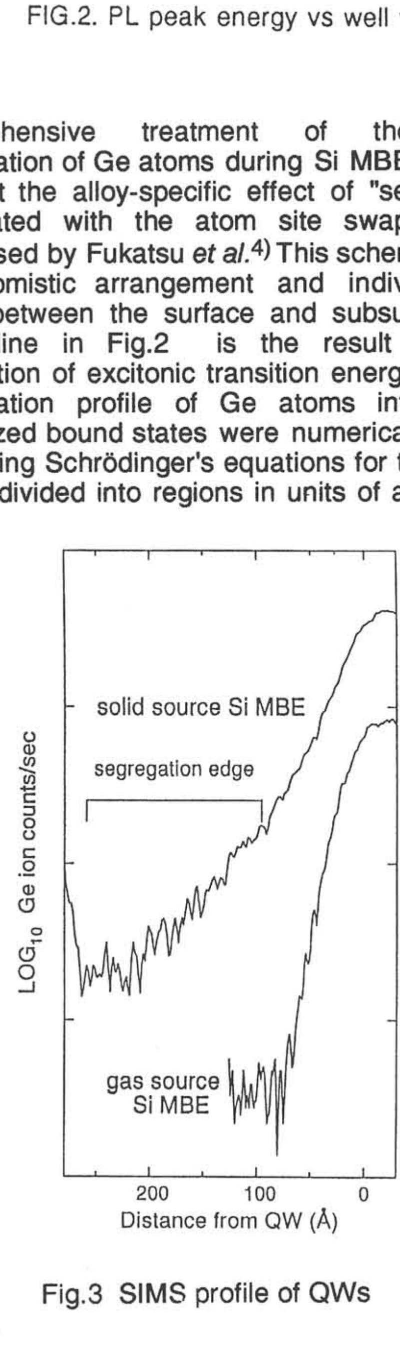

Fig.3 SIMS profile of QWs

Ground state energies in conduction and valence bands were obtained by matching the wavefunction and its first derivative at the interface of neighboring regions. The calculation is in close agreement with the experiment when we use segregation potential Eb, i.e. the energy deficit of the surface state to the subsurafce state, of 0.28±0.3meV. If we choose Eb as a fitting parameter instead, Eb=0.25meV is obtained by a least-squares fit and the difference is negligible.

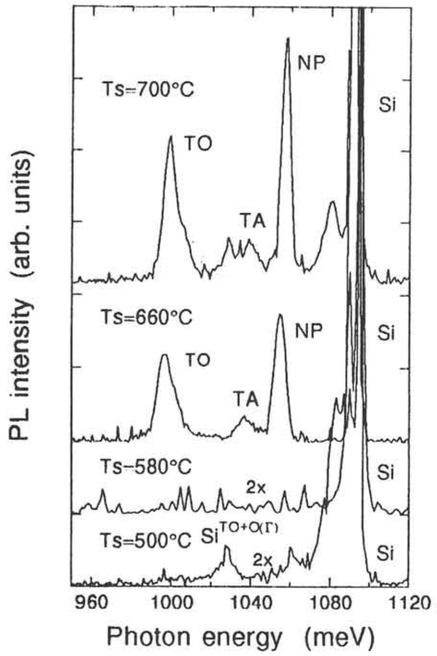

Fig.4 Growth temperature dependence of PL spectra

To strengthen our idea that high growth temperature environment is a critical issue which dictates the PL efficiency, we performed PL study of SiGe/Si SQWs with well width of 50Å grown at different growth temperatures 500 - 700 °C. As shown in Fig.4, no band edge emission from QW layers was observed in 500 °C grown sample. In contrast, higher temperature (Ts>600 °C) employed samples exhibited distinct band edge emission. It should be noted that deep level emissions characteristic to poor crystallinity cannot be seen. Since usual strained-layer growth is kinetic, where adatom motions are hampered and not equilibrated, lattice imperfections such as point defects and local lattice distortion are likely to be introduced. Present result clearly shows that the choice of a higher growth temperature is essential to efficient luminescence within a scheme of enhancing mobility of adatoms. This is in agreement with a recent study of GS-Si MBE that the emission efficiency is reduced when the growth temperature is lowered below the optimum temperature only by 10°C. So we can conclude that the selection of high growth temperature to improve the quality of crystallinity is the most crucial point for radiative recombination.

4. Conclusion

We succeeded in growing highly luminescent $Si_{0.8}Ge_{0.2}/Si$ single quantum well structures by conventional "solid source" Si MBE. Well width dependence of the transition energy was well explained by potential distortion due to Ge surface segregation during growth. The choice of high growth temperature, Ts>600°C, beyond the conventional temperature window, 400-600°C, was found to be essential to luminescent layer growth.

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