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Formation of Luminescent $Si_{1-x}Ge_x$/Si Quantum Wells with Abrupt Interfaces by Segregant-Assisted Growth

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We report the formation of luminescent $Si_{1-x}Ge_x$/Si quantum wells (QWs) with abrupt interfaces by segregant-assisted growth (SAG) technique using an Sb adlayer. Systematic photoluminescence (PL) study revealed that SAG-grown samples show spectral red-shift compared to those grown by conventional solid-source molecular beam epitaxy (MBE) due to the sharp Si/$Si_{1-x}Ge_x$ interface. Electroluminescence (EL) was observed from a $Si_{1-x}Ge_x$/Si *p-i-n* diode formed by utilizing Sb incorporation during SAG.

1. Introduction

To obtain an abrupt interface is one of the most serious problems in the field of band engineering. Particularly, in SiGe/Si system grown by molecular beam epitaxy (MBE) , it is difficult to realize the abrupt interfaces due to the surface segregation of Ge atoms. In order to realize subnanometer interfacial controllability, Copel *et al.* demonstrated a new growth technique based on altering the energetics of growth using a "surfactant" and showed successful reduction of islanding formation and interfacial mixing using As surfactant layer[1]. Fujita *et al.* adopted submonolayer of Sb, the most useful n-type dopant in Si, as a surfactant, and demonstrated the suppression of surface segregation of Ge atoms and formation of Si/Ge superlattices with abrupt interfaces using x-ray photoelectron spectroscopy (XPS) and secondary ion mass spectrometry (SIMS)[2]. They named this growth technique as "segregant assisted growth (SAG)" after the tendency of Sb which shows strong segregation in Si[3]. Our previous report showed that Ge surface segregation distorts the potential profile of SiGe/Si quantum wells (QWs), resulting in a significant blue-shift in photoluminescence (PL) spectra compared to the calculated result using a rectangular profile[4]. This segregation-induced spectral blue-shift is expected to be removed by SAG. However, systematic study on the formation of luminescent QWs by SAG was lacking. In this paper, we report the formation of luminescent $Si_{1-x}Ge_x$/Si QWs with abrupt interfaces by SAG using an Sb adlayer.

2. Experimental

All the growth were started after a conventional pretreatment of a Si substrate which generates a protective oxide layer. Si was evaporated from an electron beam evaporator with the flux controlled by a crystal oscillator. Ge and Sb were evaporated by effusion cells. Following a 2000Å buffer layer grown at 800°C, growth temperature was lowered to 620°C. This growth temperature is enough high to obtain luminescent quantum well layers. 0.75 monolayer of Sb was deposited at the top interface (after growth of $Si_{1-x}Ge_x$ well layer) in order to avoid the incorporation of segregant in the well layer. The amount of Sb was chosen so as not to lose the quality of crystallinity. After overlayer growth, short thermal treatment at 800°C for 10 minutes was performed to remove the residual Sb floating up to the surface. The sample structure and the growth sequence are summarized in Figure 1. For the electroluminescence (EL) study, mesa diode structures were created by chemically etching down through Si substrate, leaving circular columns of 500μm in

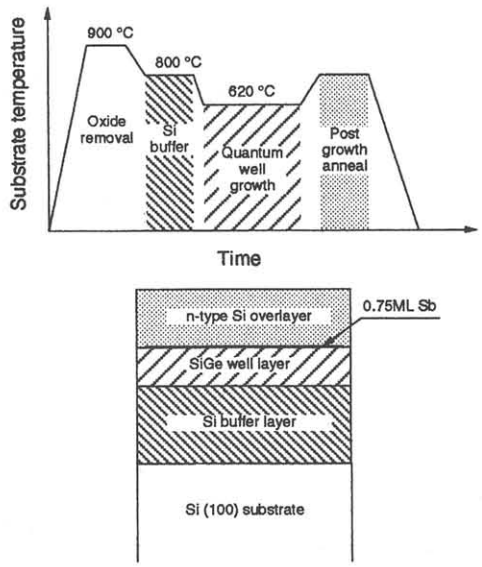

Fig.1 Typical growth temperature profile for SAG operation and the sample structure.

diameter, using a mixture of hydrofluoric acid (HF) and nitric acid (HNO_3) of 1:10. No protective oxide films was deposited after mesa fabrication. Thin aluminum layer was deposited by conventional vacuum evaporation for electrical contact. PL and EL were recorderd in standard lock-in configuration and detected by a liquid-nitrogen-cooled Ge photodetector. Excitation was provided by a defocused argon ion laser.

3. Results and Discussion

Figure 2 shows PL spectra of $Si_{1-x}Ge_x/Si$ SQW structures with well width of 30Å grown by conventional SSMBE without Sb adlayer and under SAG operation. Phonon-resolved spectra can be obtained in the both spectra. Interestingly, transition energy can be seen to shift to lower energy side than that of the sample grown without Sb. This remarkable shift was brought by the formation of abrupt Si/SiGe interfaces, which was checked by sputter depth profiling.

As shown in Fig.3, systematic variation of well width shows quantum confinement effect which can be explained by ideal square potential profile. Solid circles are the experimental results of SQWs grown without Sb adlayer, and solid triangles belong to the SAG grown samples. The calculated transition energy taking Ge surface segregation is shown in solid line. The calculation was carried out by solving Schrödinger's

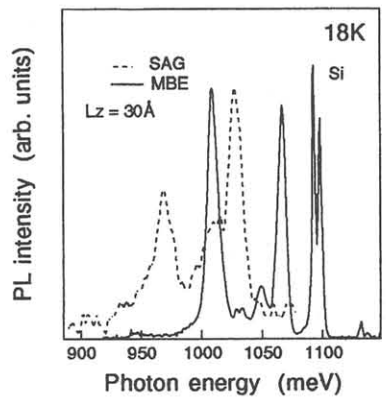

Fig.2 PL spectra of $Si_{0.8}Ge_{0.2}/Si$ SQW structures.

equations for the potential profile numerically obtained in units of atomic layer from the model invoiving the effect of "self-limitation"[5),6)]. The broken line shows the theoretical result assuming a standard square potential profile. Although the agreement between numerical and experimental results is pretty good, we notice that NP transition energy is smaller than the calculated value using a square well potential. This is probably due to high Ge concentration layer at top interface frozen by Sb adlayer and/or built-in potential brought by incorporation of Sb into Si overlater.

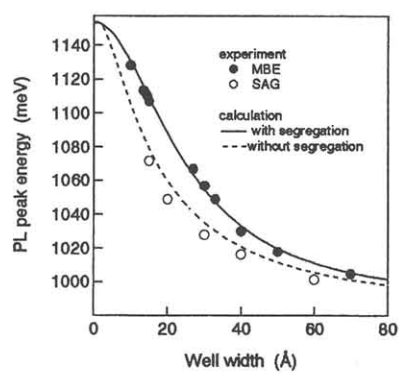

Fig.3 Well width dependence of NP transition energy.

Fabrication of light emitting $Si_{1-x}Ge_x/Si$ diode by SAG was also investigated. Since a part of Sb is incorporated into Si overlayer during growth, n-type Si cap layer is formed without any dopant coevaporation. From the *p-i-n* $Si_{1-x}Ge_x/Si$ diode structure on a p-type Si substrate, intense electroluminescence (EL) was observed at 18-90K as shown in Fig.4. This demonstrates that the Sb SAG offers us two fold advantages of producing a sharp compositional transition and the feasibility of giving a top degenerate n-type contact layer.

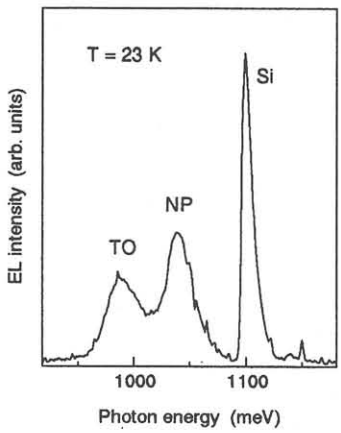

Fig.4 Electroluminescence from a SAG-grown SiGe/Si single quantum well structure.

4. Conclusion

We succeeded in the formation of luminescent SiGe/Si quantum wells with abrupt interfaces by segregant-assisted growth. Spectral red-shift was observed due to the abrupt compositional transirion due to Sb adlayer. Electroluminescence was also observed from the *p-i-n* $Si_{1-x}Ge_x$/Si diode structure on a p-type Si substrate.

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