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Local-Symmetry Induced Light Emission from $Si/Si_{1-x}Ge_x/Si$ Quantum Wells

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To clarify how the light emission from pseudomorphic $Si/Si_{1-x}Ge_x/Si$ quantum wells is affected by the microscopic structures of $Si_{1-x}Ge_x$ alloys, the photoluminescence of $Si/Si_{1-x}Ge_x/Si$ under [110] uniaxial tensile stress was investigated. The intensity of no-phonon light emission has an anomalous dip at a certain strain field. This suggests that recovering of the tetrahedral symmetry in a $Si_{1-x}Ge_x$ alloy decreases the light emissivity of $Si/Si_{1-x}Ge_x/Si$, since the existing bi-axial strain created during molecular beam epitaxial (MBE) growth is relaxed by applying a stress. Moreover, $Si/Si_{1-x}Ge_x/Si$ quantum wells were fabricated by MBE using atomic hydrogen (H^+) irradiation to control the precipitation of Ge atoms in the $Si_{1-x}Ge_x$ alloy, and enhanced light emissivity of the $Si/Si_{1-x}Ge_x/Si$ grown with H^+ irradiation was observed. These results suggest that the local symmetry around Ge influences the light emissivity of $Si/Si_{1-x}Ge_x/Si$ quantum wells.

1. Introduction

Intense photoluminescence (PL) due to no-phonon transition has been obtained from $Si_{1-x}Ge_x$ layers [1]. This phenomenon has been explained with an "alloy model", where the alloy randomness in a $Si_{1-x}Ge_x$ layer breaks the Bloch state. However, recent calculations [2], which were based on a first-principle molecular dynamic technique, showed that the local symmetry of Si-Ge bonds plays an important role in the light emission. To verify this effect, we fabricated $Si/Si_{1-x}Ge_x/Si$ quantum wells by solid source molecular-beam epitaxy (SS-MBE) with and without atomic hydrogen (H^+) irradiation so that we could control the precipitation of Ge atoms in a $Si_{1-x}Ge_x$ alloy. This is possible because H^+ irradiation during MBE growth plays a role in suppressing surface segregation [3] and diffusion [4]. We also measured the PL spectrum under uniaxial [110] tensile stress to investigate how the light emissivity of $Si/Si_{1-x}Ge_x/Si$ is affected by the circumstantial microscopic structure.

2. Experimental

$Si/Si_{1-x}Ge_x/Si$ structures were grown on Si(001) with an SS-MBE system that consists of an electron gun evaporator to deposit Si, a Knudsen-cell to deposit Ge, and a gas cell to introduce atomic hydrogen. Atomic hydrogen was formed by applying RF power to the gas cell. The ratio of atomic hydrogen to the total flow was nominally 0.5%, and the rate of its irradiation was 20 ML/s (1 ML=6.78×10^{14} cm^{-2}). A 50-nm-thick pseudomorphic $Si_{1-x}Ge_x$ layer was grown at 300℃ to form abrupt $Si_{1-x}Ge_x/Si$ interfaces, and a 100-nm-thick Si buffer and a Si cap layer were grown at 600℃. After MBE growth, the $Si/Si_{1-x}Ge_x/Si$ samples were annealed at 900℃ for 15 minutes in a N_2 ambient using a conventional furnace to eliminate the point defects generated by low temperature growth in the quantum wells. The alloy compositions were determined by X-ray diffraction using (004) diffraction of CuKα radiation.

A schematic illustration of the sample holder we used for the observations of PL under uniaxial stress is shown in Fig. 1. The $Si/Si_{1-x}Ge_x/Si$ samples were placed in a cantilevered geometry. The left end of the sample was fixed, while the right end was pushed by a driving screw. As a result, a uniaxial strain field was introduced into the sample surface along the [110] direction. Since the strain field varied linearly along the [110] direction, the strain field dependence of the PL spectra could be obtained by moving the spot position where the Ar^+ laser (spot diameter: 0.5 mm) was irradiated.

3. Results and Discussion

Typical PL spectra of a $Si/Si_{0.8}Ge_{0.2}/Si$ structure under [110] uniaxial stress at 4.2 K are shown in Fig. 2. As the uniaxial stress increased, the PL peaks from the Si substrate (Si(TA) and Si(TO)) shifted towards the lower energy side and peaks from the $Si_{1-x}Ge_x$ layer (SiGe(NP) and SiGe(TO)) shifted towards the higher energy side. From the slope of the PL peak (SiGe(NP)) shift vs. strain curve, we derived the deformation potential. The deformation potentials of the $Si_{1-x}Ge_x$ layers ($0.08 \le x \le 0.23$) were almost constant (15 meV/GPa) as observed by Houghton et al.[5].

The peak intensity of PL due to no-phonon transition is summarized in Fig. 3 as a function of the [110] tensile strain (ε). An anomalous dip is seen at a certain strain field (ε=0.03%). The PL intensity decreases by recovering from the asymmetry of the $Si_{1-x}Ge_x$, since the strain created during molecular beam epitaxial (MBE) growth is relaxed by applying a stress. When the stress field exceeds a critical value (ε=0.03%), the symmetry of the $Si_{1-x}Ge_x$ alloy begins to fall. As a result, the PL intensity increases with the increase in tensile stress.

To control the distribution of Ge atoms in $Si_{1-x}Ge_x$ alloy and the local symmetry of the Si-Ge bond in the $Si_{1-x}Ge_x$ alloy, we used surfactant epitaxy, where atomic hydrogen was irradiated during the SS-MBE growth. In this way, the precipitation of Ge atoms could be controlled through the H^+ dose and the growth temperature. The results shown in Fig. 4 clearly show that the light emissivity is improved by using the surfactant epitaxy under tensile stress. The saturation of intensity under a large strain field in a Ge-precipitated alloy can be attributed to by the relaxation of strain on the Si-Ge bond due to the strain on the Ge-Ge bond, since the strength of the Si-Ge bond is greater than that of the Ge-Ge bond. These results suggest that the strain field does not spread throughout the $Si_{1-x}Ge_x$ lattice uniformly. In other words, the strain field is locally confined near the Ge atoms.

Therefore, the local symmetry appears to have an important effect on the light emission from $Si/Si_{1-x}Ge_x/Si$ quantum wells.

4. Summary

We have investigated photoluminescence from $Si/Si_{1-x}Ge_x$ fabricated by SS-MBE with and without H^+ irradiation under [110] uniaxial tensile stress at 4.2 K. The intensity of no-phonon light emission has an anomalous dip at a certain strain field. This suggests that recovering of the tetrahedral symmetry in a $Si_{1-x}Ge_x$ alloy decreases the light emissivity of $Si/Si_{1-x}Ge_x/Si$. Enhanced light emissivity of $Si/Si_{1-x}Ge_x/Si$ grown with H^+ irradiation was observed. Decreasing the strain on the Si-Ge bond through the precipitation of Ge in a $Si_{1-x}Ge_x$ alloy appears to decrease the light emissivity from $Si/Si_{1-x}Ge_x/Si$. Therefore, the local symmetry of the $Si_{1-x}Ge_x$ influences the light emissivity of $Si/Si_{1-x}Ge_x/Si$ quantum wells.

5. Acknowledgment

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6. References

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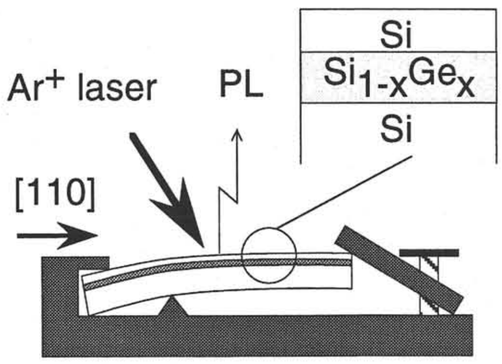

Fig. 1 A schematic of the sample holder for PL observations under uniaxial stress

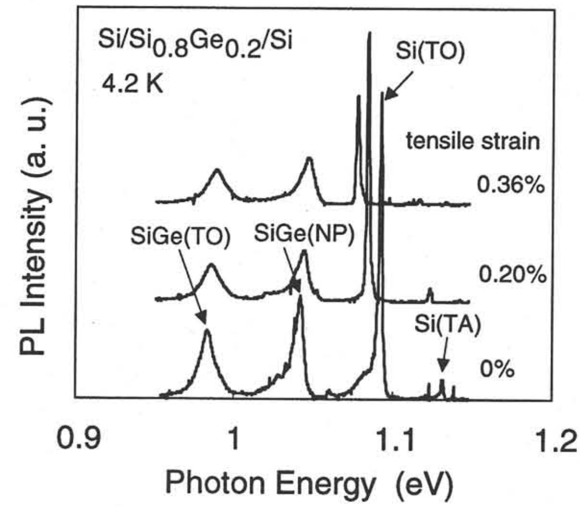

Fig. 2 PL spectra under [110] tensile strain

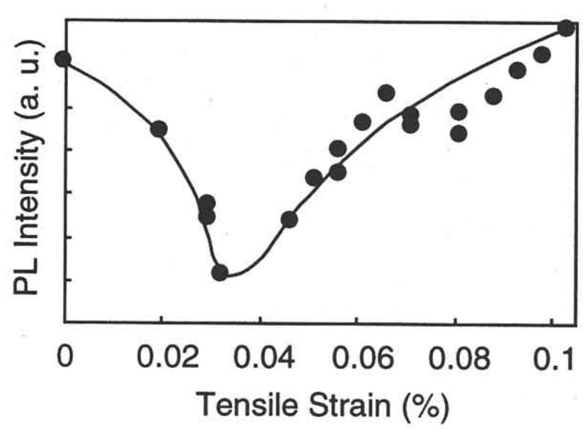

Fig. 3 PL intensities (SiGe(NP)) from the $Si_{0.8}Ge_{0.2}$ layer as a function of [110] tensile strain

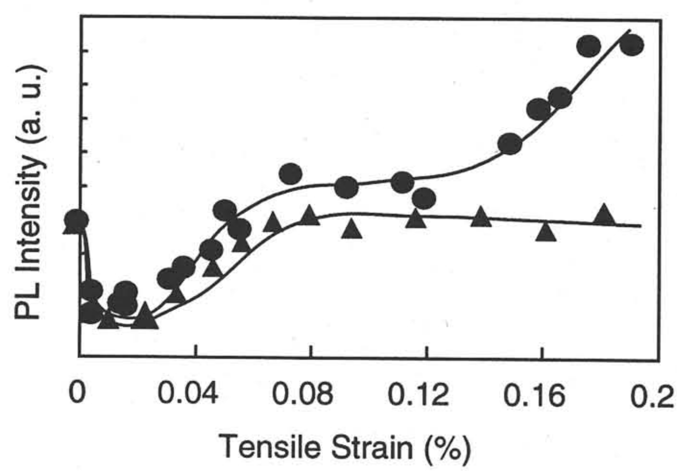

Fig. 4 PL intensities (SiGe(NP)) from the $Si/Si_{0.82}Ge_{0.18}/Si$ layer fabricated by MBE (triangles) and surfactant epitaxy (circles) as a function of [110] tensile strain.