Quantitative Correlation between the Surface Segregation of Ge and the Light Emission of Si/SiGe/Si Heterostructures

Yoshinobu Kimura, Kiyokazu Nakagawa and Masanobu Miyao

Central Research Laboratory, Hitachi, Ltd., Kokubunji, Tokyo 185, Japan Phone: +81-423-23-1111, Fax: +81-423-27-7722, E-mail: yoshinob@crl.hitachi.co.jp

1. Introduction

There have been many investigations into the band edge luminescence from strained $Si/Si_{1-x}Ge_x/Si$ quantum wells, aimed at realizing Si-based optoelectronic integrated circuits [1]. Intense no-phonon light emission can be realized by using the indirect band gap materials Si and Ge due to the alloy randomness, and this emission does not follow the momentum conservation rule for optical transition [2]. However, the quantitative correlation between crystal growth conditions and luminescence intensity has not been clarified.

Recently, we reported that the photoluminescence (PL) intensity was very weak when Si/SiGe/Si was grown within a specific temperature range (400°C - 700°C) [3]. Since this temperature range corresponds to the region where the surface segregation of Ge is active during MBE growth [4], the surface segregation length is likely to be an important factor in determining the level of PL intensity.

In this paper, we examine the control of Ge surface segregation by using atomic hydrogen (H) assisted molecular beam epitaxy (MBE). A quantitative relation between the surface segregation length of Ge and the PL intensity is determined.

2. Experimental

We grew Si/Si_{1-x}Ge_x/Si ($0.12 \le x \le 0.16$) heterostructures on a Si(001) substrate. A 100-nm-thick Si buffer layer was grown at 600°C, and a 50-nm-thick Si_{1-x}Ge_x layer was grown with or without H irradiation at temperatures (Tg) ranging from 300 to 600°C. A 50-nm-thick Si cap layer was grown over the Si_{1-x}Ge_x layer at 600°C, and finally, all the samples were annealed at 900°C for 3 hours in a N₂ ambient.

The PL spectra of the Si/Si_{1-x}Ge_x/Si samples were measured with a conventional PL setup at 4.2 K. The surface-excitation source was a 100-mW Ar ion laser (wavelength: 514.5 nm).

The surface segregation length of Ge was evaluated by measuring the surface Ge concentration during Si MBE with x-ray photoelectron spectroscopy (XPS), where a Si layer was successively deposited on a Si(001) substrate covered with a with Ge layer less than 1ML thick (1 ML: 6.78×10^{14} atoms/cm²). The Ge segregation length was defined as the deposited Si thickness at which the surface concentration of Ge becomes 1/10 of the initial Ge concentration.

3. Results and Discussion

Figure 1 shows the PL spectra of Si/Si_{0.85}Ge_{0.15}/Si (Tg: 400°C) without H irradiation (a), and with H irradiation (b). The irradiation rate during MBE growth was 0.3 ML/s. The two main peaks of the SiGe layer are labeled NP and TO, where NP refers to a no-phonon transition and TO refers to a TO-phonon replica due to the Si-Si mode. The use of H irradiation increased the peak intensities of both NP and TO as shown in the inset.

The growth temperature dependence on NP intensity is shown in Fig. 2, where the H irradiation rate is used as a parameter. For the samples grown without H irradiation, PL intensity was low at above 400°C. On the other hand, PL intensities for the samples grown with H irradiation (0.6 ML/s) shows a maximum value at 400°C. These intensities decreased above 400°C, which we attribute to the diminishing number of surface terminating hydrogen atoms.

We obtained the surface segregation length (Ls) of Ge on the Si (001) surface as a function of growth temperature (the inset in fig. 2). The surface segregation length from 400 $^{\circ}$ C to 500 $^{\circ}$ C was much lower when atomic hydrogen irradiation was used compared to the surface segregation length without the irradiation.



Fig. 1 Photoluminescence spectra of $Si/Si_{0.85}Ge_{0.15}/Si$ at 4.2 K, (a) without H irradiation, (b) with 0.3 ML/s of H irradiation during molecular beam epitaxy. Photoluminescence intensity of SiGe is shown as a function of the H irradiation rate in the inset.



Fig. 2 Photoluminescence intensity of NP plotted against growth temperature of the $Si_{0.85}Ge_{0.15}$ layer. The surface segregation length of Ge on the Si(001) is plotted against growth temperature in the inset.

We obtained the quantitative relation between the PL intensity (NP) and the Ge segregation length from Fig. 2 and it is shown in Fig. 3. The intensity of NP increased as Ls decreased, and when the surface segregation length of Ge was less than 7 nm, the PL intensity increased drastically. These results clearly indicate that the surface segregation length of Ge is a key parameter that helps determine the light emission from SiGe.

To investigate the effects of the Ge surface segregation, we plotted the PL intensity ratio between TO and NP against x, (fig. 4). From a simple statistical calculation [5], we



Fig. 3 Photoluminescence intensity of NP as a function of Ge segregation length. The open symbols refer to the samples grown with H, and the filled symbols refer to the samples grown without H.



Fig. 4 The intensity ratio of TO to NP as a function of the Ge composition x. A theoretical curve for an ideal random alloy is shown by the solid curve. The data fit well with the curve only for the sample with high PL intensity.

determined that the intensity ratio (TO/NP) is proportional to 1/[x (1-x)] in the case of an ideal random alloy. Our experimental results indicated that the TO/NP ratio fit well with the theoretical curve (the solid curve in Fig. 4) for the samples with a short surface segregation length (Ls < 7 nm). On the other hand, the TO/NP ratio for the samples with a long surface segregation length (Ls \geq 7 nm) deviated noticeably from the theoretical curve. These results suggest that the light emission originates from Si-Ge bonds and its intensity decreases when Ge distribution deviates from the ideal random alloy because an excess Ge-Ge bonds form.

4. Conclusions

The quantitative relation between the PL intensity of SiGe and the Ge surface segregation length was obtained. Intense PL is obtained when the surface segregation length is suppressed to less than 7 nm by H irradiation. When the surface segregation phenomena become active (Ls > 7 nm), PL intensity decreases drastically. We attribute this to the deviation of the Ge distribution from that of an ideal random alloy.

References

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