Growth and Characterization of Si-Based Light-Emitting Diode with β-$FeSi_2$ Active Region by Molecular Beam Epitaxy

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Abstract- **Si *p-n* junction light-emitting diodes with β-$FeSi_2$ particles and with a β-$FeSi_2$ continuous film active region were grown on Si(001) and Si(111) substrates, respectively, by molecular beam epitaxy and the electroluminescence properties were investigated.**

I. INTRODUCTION

β-$FeSi_2$ has been attracting much attention as a Si-based light emitter with a wavelength (1.5 μm) corresponding to optical fiber communication [1]. In 1997, Leong *et al.* reported the low-temperature electroluminescence (EL) from β-$FeSi_2$ precipitates embedded in a Si *p-n* junction by ion beam synthesis (IBS) [2]. However, room temperature (RT) EL has been difficult to obtain due to a large number of induced defects. We therefore adopted reactive deposition epitaxy (RDE; deposition of Fe on a hot Si) instead of IBS to form β-$FeSi_2$, and developed the formation technique of single-crystalline β-$FeSi_2$ particles embedded in Si by molecular beam epitaxy (MBE), leading to the first RT 1.6 μm EL [3,4]. The problem is, however, the fact that active region is not a continuous β-$FeSi_2$ film but particles. From the viewpoint of carrier injection into β-$FeSi_2$, a continuous active layer is favorable. However, the epitaxial β-$FeSi_2$ film on Si(001) was found to easily aggregate into isolated islands due to the lattice mismatch (1–2 %) between the two materials when it was annealed at high temperature for improving the crystalline quality or embedded by MBE-Si capping layers [5]. We have been trying to enhance EL intensity by increasing the size of β-$FeSi_2$ particles in Si, but it was found to just increase the defect densities in surrounding Si [6]. On the other hand, there have been a few reports showing that smooth β-$FeSi_2$ films can be grown on Si(111), even at high temperatures, in spite the large lattice mismatch (~5 %) between the two materials [7,8]. To the best of our knowledge, there have been no reports of the formation of a Si/β-$FeSi_2$/Si double heterostructure (DH) by MBE.

In this paper, we have reported that fabrication of multiple β-$FeSi_2$-particles/Si layered structure is a very effective way to enhance EL from *p*-Si/β-$FeSi_2$-particles/*n*-Si light-emitting diodes (LEDs). EL from *p*-Si/β-$FeSi_2$ film/*n*-Si DH structures formed on Si(111) substrates by MBE was also demonstrated for the first time.

II. EXPERIMENTAL

β-$FeSi_2$-particles/Si multilayered structure was fabricated on Si(001) as follows. First, [100]-oriented β-$FeSi_2$ epilayers were grown on n^+-Si(001) substrates by RDE at 470°C. The sample was then annealed *in situ* at 850°C for 1 h to improve the crystal quality of the β-$FeSi_2$. The β-$FeSi_2$ film agglomerated into islands during this process, due to the lattice mismatch (1–2 %) between the two materials [5]. Consequently, a 0.3 μm-thick undoped Si layer was grown by MBE at 500°C. This process was repeated for double- and triple-layered structures. After embedding β-$FeSi_2$ in Si, a boron-doped p^+-Si capping layer was grown at 700°C. Samples were finally annealed at 900°C in an Ar atmosphere for 14 h to further improve the crystal quality, resulting in β-$FeSi_2$ particles embedded in Si matrix.

For LEDs on Si(111), a 20 nm-thick β-$FeSi_2$ epitaxial layer was grown by RDE at 650°C as a first step, and this layer was used as a template. Next, a 70 nm-thick undoped β-$FeSi_2$ layer was epitaxially grown by MBE at 750°C, followed by a 0.5 μm-thick undoped MBE-Si overlayer grown at 500°C. Finally, a 0.2 μm-thick boron-doped p^+-Si capping layer was grown at 700°C. To improve the crystal quality, the wafer was annealed in Ar at 800°C for 14 h.

The mesa structure of 1.5×1.5 mm^2 was made by wet chemical etching. The EL spectra were measured under 200 Hz pulsed current biasing of 50 % duty cycle. Luminescence was dispersed by a 25cm focal-length grating monochromator, and detected phase sensitively by a liquid nitrogen cooled InP/InGaAs photomultiplier (Hamamatsu Photonics R5509-72).

III. RESULTS ANS DISCUSSION

A. LED on Si(001)

Cross-sectional SEM images of single-, double- and triple-layered β-$FeSi_2$-particles/Si structures without the p^+-Si capping layer were shown in Figs. 1(a),

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1(b) and 1(c), respectively. We can see clear layered structure of β-$FeSi_2$ particles in these samples. It was found from θ–2θ X-ray diffraction spectra that the epitaxial relationship between the β-$FeSi_2$ and Si was preserved even after the aggregation and the Si overgrowth.

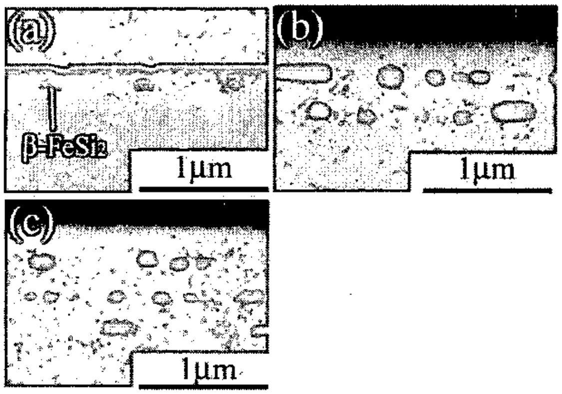

Fig.1 SEM cross sections of (a) single-, (b) double- and (c) triple-layered β-$FeSi_2$-particles/Si structures.

Figure 2 shows photoluminescence (PL) spectra measured at 77 K for these three samples. It was found that the 1.53 μm PL intensity was proportional almost to the number of β-$FeSi_2$-particles /Si layered structure. This is attributed to the fact that the number of β-$FeSi_2$ particles where electron and hole pairs recombine radiatively increased without increasing defect densities.

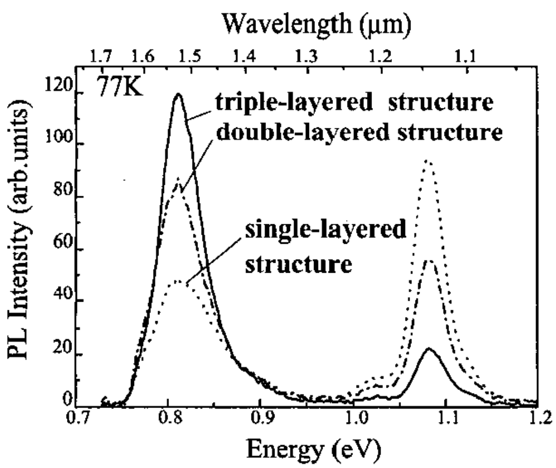

Fig. 2 PL spectra measured at 77 K.

Hereafter we compare the EL properties of a single-layered LED with those of a double-layered one. Both samples showed clear rectifying characteristics of Si *p-n* junctions in the current-voltage characteristics. RT EL spectra as a function of injected current density obtained for single-layered LED were shown in Fig.3 for reference. The 1.6 μm EL was observed for current density above 70 A/cm^2, and the EL intensity increased superlinearly with injected current as observed in our previous LEDs, probably due to nonradiative recombination centers in and around the β-$FeSi_2$ [3,4].

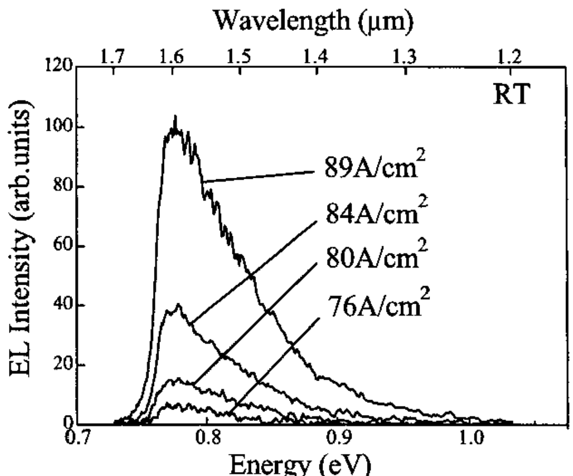

Fig. 3 RT EL spectra as a function of injected current density measured at RT.

Figure 4 shows the temperature dependence of 1.6 μm EL intensity for single- and double-layered LEDs. The EL intensity for the double-layered LED was much stronger than that of the single-layered LED, differently from the results obtained in PL. The reason for this EL enhancement has not yet been clarified, but the densities of electron and hole which recombine radiatively are much higher in the upper β-$FeSi_2$ particles than in the lower ones. By further optimizing the diode structure and the doping profile, EL intensity will be improved very much.

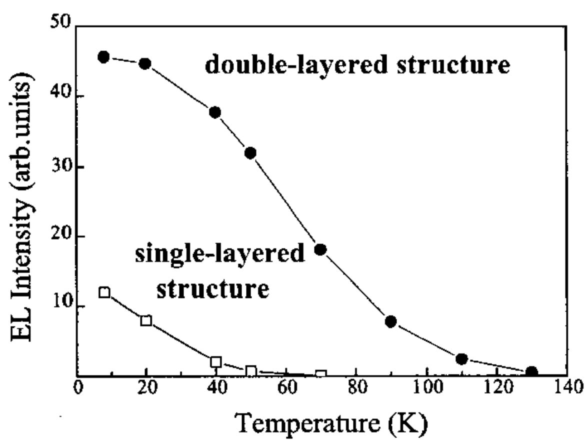

Fig. 4 Temperature dependence of integrated EL intensity.

B. *LED on Si(111)*

Figure 5 (a) shows the cross-sectional SEM image of the DH structure formed on the Si(111) substrate. The β-$FeSi_2$ continuous film was successfully embedded in a Si matrix. It was found that both the thickness of the Si overlayer and the annealing temperature were key parameters to forming a Si/β-$FeSi_2$/Si DH structure on Si(111). If the annealing temperature was higher (~900°C) or the thickness of the Si overlayer was thinner (~0.3 μm), β-$FeSi_2$ was found to aggregate into particles during high temperature annealing as shown in Fig. 5(b). This aggregation is due probably to the lattice mismatch between the two materials. For reference, a typical example of Si/β-$FeSi_2$ particles/Si structure formed on Si(001) is shown in Fig. 5 (c) [6].

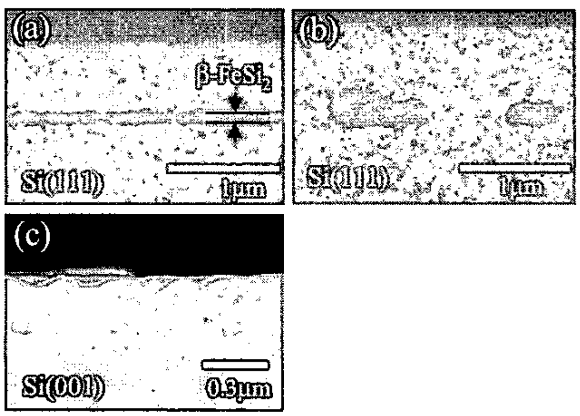

Fig.5 Cross sectional SEM images of Si/β-$FeSi_2$/Si structures on Si(111) obtained after annealing at (a) 800°C and (b) 900°C. (c) is a typical example of Si/β-$FeSi_2$/Si structure formed on Si(001).

Figure 6 shows EL spectra as a function of injected current density at 77K. The EL peak was observed at approximately 1.55 μm at low current injection, but it showed clear blue shift with increasing injected current density. This is due probably to the band-filling effect. When the bias current is large enough, ground states are occupied and injected carriers start to fill the higher energy levels, giving rise to EL with higher peak energy. It was also found that the integrated EL intensity of the LED increased almost linearly with injected current density as shown in the inset of Fig. 6. This result suggests that most of the bias current contributed to the EL from the embedded β-$FeSi_2$ active layer. Our first, non-optimized LED showed weak but observable EL at RT. We therefore suppose that by optimizing the growth condition and the doping profile, practical Si-based LEDs will be obtained in the near future.

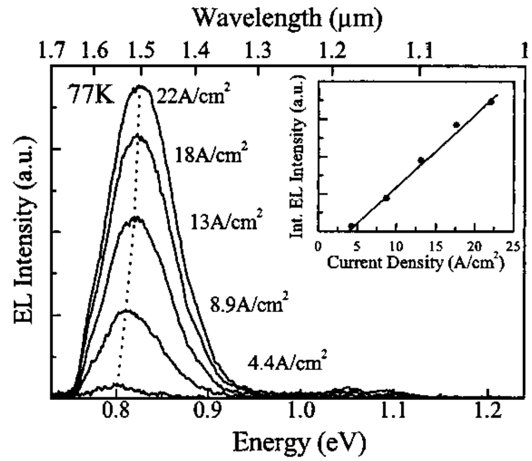

Fig. 6 EL spectra at 77 K. Inset is the current density dependence of integrated EL intensity.

IV. CONCLUSION

We have fabricated Si-based LEDs with β-$FeSi_2$ particles active region and found that the multilayered LED structure was very effective to enhance the RT 1.6μm EL. We have also fabricated DH structure LEDs with a β-$FeSi_2$ film active region on Si(111) substrate by MBE. It was found that both the thickness of the Si overlayer and the annealing temperature were key parameters to forming a Si/β-$FeSi_2$/Si DH structure on Si(111) without aggregation of β-$FeSi_2$.

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